

Time as an observable in nonrelativistic quantum mechanics

G. E. Hahne*
NASA, Ames Research Center
Moffett Field, California, 94035 USA

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Abstract

The argument follows from the viewpoint that quantum mechanics is taken not in the usual form involving vectors and linear operators in Hilbert spaces, but as a boundary value problem for a special class of partial differential equations—in the present work, the nonrelativistic Schrödinger equation for motion of a structureless particle in four-dimensional space-time in the presence of a potential energy distribution that can be time- as well as space-dependent. The domain of interest is taken to be one of two semi-infinite boxes, one bounded by two t =constant planes and the other by two z =constant planes. Each gives rise to a characteristic boundary value problem: one in which the initial, input values on one t =constant wall are given, with zero asymptotic wavefunction values in all spatial directions, the output being the values on the second t =constant wall; the second with certain input values given on both z =constant walls, with zero asymptotic values in all directions involving time and the other spatial coordinates, the output being the complementary values on the z -constant walls. The first problem corresponds to ordinary quantum mechanics; the second, to a fully time-dependent version of a problem normally considered only for the steady state (time-independent Schrödinger equation). The second problem is formulated in detail. A conserved indefinite metric is associated with space-like propagation, where the sign of the norm of a unidirectional state corresponds to its spatial direction of travel. The time t , its conjugate momentum $p_t = -i\hbar\partial/\partial t$, and its momentum-space form $i\hbar\partial/\partial p_t$, appear as operators in the space of states. A theory of average dwell and delay times in the interaction of a particle with a generic time-dependent potential barrier is proposed. Analytic results are obtained for the simple case of a step potential barrier. The problems of calculating dwell and delay times in first-order perturbation theory are treated in an appendix.

*email: gahne@mail.arc.nasa.gov

1 Introduction

Within a few years after the discovery of quantum mechanics a consensus formed (von Neumann [1], p. 188 and [2], p. 354, Pauli [3], p. 140, footnote, and [4], p. 63, footnote) to the effect that, in contrast to spatial positions, and therefore in conflict with special relativity, the temporal position t is necessarily a c-number, or parameter, with no generic operator status being mathematically feasible. In the decades intervening since the publication of the original versions of the two cited treatises in 1932 and 1933, respectively, the prohibition on specifying the time as a dynamical variable has been widely upheld as part of the standard doctrine of quantum mechanics—see, e. g., Peres [5] Chap. 12-7 and Omnes [6] p. 57. In recent decades interest in this subject has intensified, due in part to applications of tunneling phenomena in semiconductors ([7], [8] Ch. 3.2.3), and a substantial set of results has been published that introduce formalisms that argue for, or against, various quantum-mechanical definitions of time, including tunneling times, dwell times, delay times, and arrival times. For definitions, reviews, and citations, see Refs. [9], [10], [11], [12], and a collection of articles in [13].

In this paper we shall consider only the nonrelativistic form of quantum mechanics, restricted to the problem of determining the wave function of a massive, structureless particle in Galilean four-dimensional space-time in the presence of a given space- and time-dependent potential energy distribution. We shall treat quantum mechanics as a boundary-value problem for the Schrödinger equation: the specified boundary values will be regarded as input to the problem, and the derived interior values and complementary boundary values will be considered as the overall output.

Since the Schrödinger equation is of first order in time and of second order in the spatial coordinates, it is, mathematically speaking, necessary and sufficient to supply wave function values on one $t=\text{constant}$ surface, and a suitable combination of wave function and normal-derivative values on each of two $z=\text{constant}$ boundary surfaces, to infer that an interior solution exists and is unique, as discussed in Ref. [14], Ch. 5, §3. (Our mathematics differs from Friedman's in that we shall administer nonlocal boundary conditions, which distinguish input from output signals, on the spatial boundaries.) Conventional time-dependent quantum mechanics for the most part deals with specifying initial, or (but not and) occasionally final, values on a $t=\text{constant}$ surface and simple (often, zero) values on the spatial boundaries, which can be partly or wholly at infinity. Nontrivial spatial boundary values, as incoming wave amplitudes in a scattering problem, are conventionally specified only in the context of the time-independent Schrödinger equation. In the present work we shall generalize the latter problem by considering general time-dependent, as well as space-dependent, input values on spatial boundaries, in the presence of explicit time dependence in the potential energy function in the differential equation itself. We shall hereinafter denote these cases of boundary value problems as Type I and Type II, respectively. These correspond, roughly and respectively, to the first and second initial-boundary value problems analyzed in Ref. [14],

Chs. 3 and 5.

In the first problem, the wave function evolves in time from given initial values, with time-independent spatial boundary values. In the second problem, we shall consider that the wave function evolves with respect to a single spatial coordinate, say the z -coordinate, such that the interior domain corresponds to a finite interval in the chosen coordinate z . Since the differential equation is of second order, determining the evolution of a wave function in a spatial direction is generally a more difficult task of analysis in both the mathematical and physical senses than one for its evolution in time. We summarize the derivation to be carried out below in terms of the following nine observations, steps, or results: (i) the space of states on any given $z = z_1$ hyperplane has a natural doubled structure in that it comprises the direct sum of the values and of the z -derivatives of the usual space of wave functions $\psi(t, x, y, z)$ at $z = z_1$; (ii) the Hamiltonian is a 2×2 matrix of operators that is derived from the ordinary Schrödinger equation; (iii) the familiar expression for the probability current density in the z -direction is used to infer the definition of a metric operator in the space of states, where now inner products include an integral over t as well as over x and y ; (iv) the metric so derived is indefinite, and the Hamiltonian is self-adjoint with respect to the metric (synonymously, pseudo-Hermitean); (v) the norm being indefinite, we shall sometimes use the term “particle presence” to denote the unit operator, the expectation value of which is the above-mentioned norm; (vi) apart from modifications needed for closed channels, the formalism can be established so that waves traveling in the $+z$ direction have positive norm, and waves traveling in the $-z$ direction have negative norm with respect to the metric; (vii) the input and output at either end of a finite spatial interval $[z_1, z_2]$ are taken to comprise, respectively, the superposition of waves traveling into, and the superposition of waves traveling out of, the interval at the initial point z_1 and at the final point z_2 (this means that there will be only outgoing scattered waves from a zone of interaction); (viii) orthonormal sets of input or of output states, transition amplitudes, and probabilities are then computed using what amounts to a Hilbert space inner product, which is derived from the indefinite metric, but depends on the wave function and its z -derivative at both z_1 and z_2 ; (ix) the dynamics yields a mapping of open-channel input into open-channel output that is unitary.

The fact that a pseudo-Hermitean Hamiltonian describes the spatial evolution of a physical system’s wave function has another concomitant: the Hamiltonian can have, as well as real eigenvalues, nonreal eigenvalues that occur in complex conjugate pairs (Gohberg, et al., [15] p. 23, Proposition 2.4). Each such pair is associated with the two wave function solutions (one rising, the other falling exponentially) for a closed channel, or classically inaccessible region for the system when it is in an associated quantum state. We shall argue that it is natural to define the direction of travel of such a wave as the direction in which it decreases exponentially—however, the simple exponential states in such a pair each have zero norm and, with proper normalization, unit overlap, which complicates the formalism. A further complication results from the circumstance that a degenerate eigenvalue of a Hamiltonian, which in simple

problems is often a zero value, requires special treatment when the Hamiltonian cannot be diagonalized by a similarity transformation, leading to the appearance of so-called “ghost” quantum states. There is more discussion on these problems below.

Formalisms for the spatial evolution of a wave function were proposed by Kijowski [16] and by Piron [17], and their work was discussed by Mielnik [18]. These two approaches differ substantially from each other and from the formalism introduced herein, as will be discussed following Eq. (11) and in Sec. 5.

The quantum mechanics describing evolution of a wave function in both directions across a spatial interval is to an extent patterned after the author’s previous work [19] on a quantum dynamics that encompasses joint bidirectional evolution of a quantum state between two temporal walls.

The remaining sections are organized as follows: In Sec. 2, we shall formulate expressions for the four-current density associated with a physical quantity, and for the local space-time density for creating or destroying that quantity in a quantum-mechanical system. We shall also show how to prescribe physically motivated boundary conditions so that the Schrödinger equation can be solved in a semi-infinite (finite in the z -direction, infinite in the t, x, y -directions) box. In Section 3 we shall propose a formalism for computing the average temporal position of the particle at both spatial walls of the box, given the spatial input and given the S -matrix deriving from a general interaction potential energy in the box’s interior. These results will then be used to compute formulas for dwell and delay times for the particle remaining within, reflecting from, or transmitted across, the box. In Section 4 we shall obtain analytic formulas for the delay times for a step potential in the z -dimension (and constant in the other dimensions). Section 5 contains a discussion of the present formalism and of previous work on the subject. An appendix analyzes the problem of dwell and delay times for a weak, transient potential energy in first-order perturbation theory.

2 Quantum-mechanical formalism

In this section we shall set up and discuss the theory that forms the “floor” of the present work. Rather than attempt to make the formalism highly general, we shall develop the argument in a particular context: the wave function solution of Schrödinger’s equation for a particle moving in the interior of a certain simple box of four-dimensional space-time. In particular, we propose a formalism and an interpretation that incorporate the wave function into an expression for the space-time “flow” density of a physical quantity, which quantity corresponds to a certain linear operator in the function space of fully time- and space-dependent wave functions. We shall argue that it is natural to regard the four-divergence of the flow as the local density of creation and destruction of that quantity at a point in space-time for the physical system in that time-dependent quantum state. Either the volume integral of the divergence, or the surface integral of the normal component of the flow vector density, therefore represents the

total amount of that quantity generated inside the space-time box. If that quantity is the time t , this integral plausibly represents the average so-called dwell time of the particle in the given box, given that the wave function is properly normalized.

Let \mathcal{B}_1 and \mathcal{B}_2 be the following open boxes in space-time:

$$\mathcal{B}_1 = \{(t, x, y, z) | t_1 < t < t_2, -\infty < x < \infty, -\infty < y < \infty, -\infty < z < \infty\}. \quad (1a)$$

$$\mathcal{B}_2 = \{(t, x, y, z) | -\infty < t < \infty, -\infty < x < \infty, -\infty < y < \infty, z_1 < z < z_2\}. \quad (1b)$$

The Schrödinger equation for $\psi(t, x, y, z)$ for a particle of mass m can be derived from a variational principle for an action \mathcal{A} , as given in Schiff ([20], p. 499), but modified to make it real:

$$\mathcal{A} = \iiint_{\mathcal{B}} dt dx dy dz \left[\frac{i\hbar}{2} \psi^* \frac{\partial \psi}{\partial t} - \frac{i\hbar}{2} \frac{\partial \psi^*}{\partial t} \psi - \frac{\hbar^2}{2m} \nabla \psi^* \cdot \nabla \psi - \psi^* V(t, x, y, z) \psi \right]. \quad (2)$$

The equations of motion are to be obtained by keeping the boundary values of ψ and ψ^* fixed, and pretending that in the interior region ψ and ψ^* can be varied independently and “arbitrarily”. The action is stationary when $\psi(t, x, y, z)$ satisfies

$$\frac{\hbar}{i} \frac{\partial \psi}{\partial t} - \frac{\hbar^2}{2m} \nabla^2 \psi + V(t, x, y, z) \psi = 0, \quad (3)$$

and $\psi(t, x, y, z)^*$ satisfies the complex conjugate equation, for all $(t, x, y, z) \in \mathcal{B}_1$ or \mathcal{B}_2 .

Henceforth when we say “solution”, we shall mean a function defined over the entire box such that it satisfies equation (3) everywhere in \mathcal{B}_1 or \mathcal{B}_2 . The linear operators representing physical quantities will normally carry a solution into another space- and time-dependent function that is not a solution, so in effect we shall deal with the more general vector space of well-behaved, complex-valued functions of space and time that need not be solutions of the Schrödinger equation.

A standard problem in conventional quantum mechanics arises if we constrain $\psi(t, x, y, z)$ to be zero on the infinite parts of the spatial boundaries of the box \mathcal{B}_1 ; that is

$$\psi(t, x, y, z) \rightarrow 0, \text{ if } |x| + |y| + |z| \rightarrow \infty. \quad (4)$$

and require that

$$\psi(t, x, y, z) \rightarrow u(x, y, z), \text{ as } t \rightarrow t_1, \quad (5)$$

where $u(x, y, z)$ is some given complex-valued function on the earlier temporal boundary of the box. As is well known, the interior values of $\psi(t, x, y, z)$, and the limiting values on the temporally later boundary of the box at $t = t_2$, are all uniquely determined by the differential equation and these input boundary conditions. The derived values are all output in a sense, but we shall often mean

by output just the subset of boundary values that were not given as input, in the present case $\psi(t_2, x, y, z)$ with $-\infty < x < \infty$, $-\infty < y < \infty$, and $-\infty < z < \infty$.

Now let us consider a problem in box B_2 such that certain information about the limiting values of $\psi(t, x, y, z)$ and $\partial\psi/\partial z(t, x, y, z)$ on the two walls $z = z_1$ and $z = z_2$ is given as input, while the wave function is supposed to tend to zero as t and/or x and/or y tend to $\pm\infty$. We want to specify just enough input information so that a solution satisfying the input boundary conditions exists and is unique. In order to accomplish this, we need to do some preliminary work. We shall not keep to a mathematically rigorous derivation, but appeal to plausibility arguments at most steps.

We now convert the above variational principle to Hamiltonian form using the methods of Goldstein ([21], Chap. 12-4), with the proviso that it is the spatial parameter z , rather than t , that is taken as the evolution coordinate for the wave function. The quantity in square brackets in (2) is the Lagrangian density \mathcal{L} . The canonical field momenta are

$$p_\psi = \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \psi}{\partial z} \right)} = -\frac{\hbar^2}{2m} \frac{\partial \psi^*}{\partial z}, \quad (6a)$$

$$p_{\psi^*} = \frac{\partial \mathcal{L}}{\partial \left(\frac{\partial \psi^*}{\partial z} \right)} = -\frac{\hbar^2}{2m} \frac{\partial \psi}{\partial z}. \quad (6b)$$

The action principle becomes

$$\mathcal{A} = \iiint_{B_2} dt dx dy dz \left[p_\psi \frac{\partial \psi}{\partial z} + \frac{\partial \psi^*}{\partial z} p_{\psi^*} - \mathcal{H}(\psi, p_\psi, \psi^*, p_{\psi^*}) \right], \quad (7)$$

where the Hamiltonian density is

$$\mathcal{H} = -\frac{2m}{\hbar^2} p_\psi p_{\psi^*} - \frac{i\hbar}{2} \psi^* \frac{\partial \psi}{\partial t} + \frac{i\hbar}{2} \frac{\partial \psi^*}{\partial t} \psi + \frac{\hbar^2}{2m} \left(\frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} + \frac{\partial \psi^*}{\partial y} \frac{\partial \psi}{\partial y} \right) + \psi^* V \psi. \quad (8)$$

The equations of motion obtained by varying ψ^* and p_ψ are a coupled set of linear equations; a complex conjugate set is obtained by varying ψ and p_{ψ^*} . We write the former equations in 2×2 matrix-operator form as follows: We first define

$$\Psi(t, x, y, z) = \begin{bmatrix} \psi(t, x, y, z) \\ p_{\psi^*}(t, x, y, z) \end{bmatrix}; \quad (9)$$

then the equations of motion can be written

$$\frac{1}{i} \frac{\partial \Psi}{\partial z} = H_{\text{sev}} \Psi, \quad (10)$$

where the Hamiltonian H_{sev} (the subscript “sev” stands for “spatial evolution”) is

$$H_{\text{sev}} = \begin{bmatrix} 0 & \frac{2mi}{\hbar^2} \\ \frac{1}{i} \left[i\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - V(t, x, y, z) \right] & 0 \end{bmatrix}. \quad (11)$$

We note that Piron [17] obtained a Schrödinger equation for a wave function's evolution along the space-like coordinate x , but Piron's wave function has one component, and the Hamiltonian is the operator derived from the classical quantity that generates dynamical motion along the x -axis. Piron thereupon obtained a general expression for the evolution in x of the average temporal position of a particle in one space dimension, but did not develop the theory further.

In the ordinary quantum mechanics derivable from the variational principle Eq. (2), the third-, or z -component of the conserved probability four-current density is ([20], p. 27)

$$J_3(t, x, y, z) = \frac{\hbar}{2im} \left(\psi^* \frac{\partial \psi}{\partial z} - \frac{\partial \psi^*}{\partial z} \psi \right). \quad (12)$$

In the present language this expression takes the form

$$J_3 = \hbar^{-1} \Psi^\dagger M \Psi, \quad (13)$$

where M is the 2×2 matrix

$$M = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}. \quad (14)$$

Note that the matrix M is Hermitean, has unit square, and has eigenvalues ± 1 , so that it can engender an indefinite metric. By inference, we make a guess for an inner product law for two z -propagating states:

$$(\Psi_1(z); \Psi_2(z)) = \hbar^{-1} \iint_{\mathbb{R}^3} dt dx dy [\Psi_1(t, x, y, z)^\dagger M \Psi_2(t, x, y, z)]. \quad (15)$$

Note that this formula has the appropriate physical dimensions, in that if $\psi_{1,2}$ have the usual dimension $\text{length}^{-3/2}$, then the above inner product is dimensionless.

We shall now argue that the above ingredients can be made into a theory of space-like evolution of a Schrödinger wave function. We shall work with the case of z -evolution of a wave function in four-dimensional space-time, but generalizations to other cases, as radial or reaction coordinates (see [22]) for the $(3N + 1)$ -dimensional space-time involved in an N -particle wave function, are formally straightforward.

Let \mathcal{S} be the space of functions of type Eq. (9), with some appropriate boundary conditions. We define the M -adjoint of a linear operator W acting on this space as that unique operator W^\dagger such that

$$(W^\dagger \Psi_1; \Psi_2) = (\Psi_1; W \Psi_2) \quad (16)$$

for all $\Psi_1, \Psi_2 \in \mathcal{S}$; in 2×2 matrix form, with W^\dagger as the ordinary Hermitean conjugate, we have

$$W^\dagger = M W^\dagger M. \quad (17)$$

If

$$W^\dagger = W \quad (18)$$

we call W pseudo-Hermitean, and if

$$W^\dagger = W^{-1} \quad (19)$$

we call W pseudo-unitary.

If W is pseudo-Hermitean and the state Ψ is suitably normalized, we want to make the plausible specification that the (necessarily real) number $(\Psi; W\Psi)$ is the expectation value of W in the state Ψ . We argue in favor of this axiom as follows: Let $x^0 = t$, $x^1 = x$, and so on. Suppose that in the conventional Schrödinger formalism, ω is some physical quantity, such as the time \tilde{t} , the spatial positions $\tilde{x}, \tilde{y}, \tilde{z}$, or the “particle presence” $\tilde{1}$ (we denote operators standing for physical parameters with a “haček” accent over the symbols). We define the four-vector “flow” density $J_\mu^{(\omega)}(t, x, y, z)$, $\mu = 0, 1, 2, 3$, of ω as

$$J_0^{(\omega)}(t, x, y, z) = \psi(t, x, y, z)^* \omega \psi(t, x, y, z) \quad (20a)$$

$$\begin{aligned} J_k^{(\omega)}(t, x, y, z) &= \frac{\hbar}{2im} \left(\psi(t, x, y, z)^* \omega \frac{\partial \psi}{\partial x^k}(t, x, y, z) \right. \\ &\quad \left. - \frac{\partial \psi^*}{\partial x^k}(t, x, y, z) \omega \psi(t, x, y, z) \right), \text{ for } k = 1, 2, 3. \end{aligned} \quad (20b)$$

We compute the four-divergence of the above vector field, assuming that ψ is a solution to Eq. (3):

$$\begin{aligned} \sum_{\mu=0}^3 \frac{\partial J_\mu^{(\omega)}}{\partial x^\mu}(t, x, y, z) &= \frac{1}{i\hbar} \psi^* [\omega, V] \psi + \psi^* \frac{\partial \omega}{\partial t} \psi \\ &\quad + \frac{\hbar}{2im} \sum_{k=1}^3 \left(\psi^* \frac{\partial \omega}{\partial x^k} \frac{\partial \psi}{\partial x^k} - \frac{\partial \psi^*}{\partial x^k} \frac{\partial \omega}{\partial x^k} \psi \right). \end{aligned} \quad (21)$$

This divergence can be construed to be the local density of creation or destruction of the quantity ω by the system in the state $\psi(t, x, y, z)$. If the divergence is zero, as for the case $\omega = \tilde{1}$, the associated quantity is not being created or destroyed and is both globally and locally conserved. More complicated situations can arise, as for $\omega = l_z = \tilde{x}\tilde{p}_y - \tilde{y}\tilde{p}_x$, the z -component of angular momentum, for a rotationally symmetric potential: The four-divergence of the current reduces to an x, y -divergence, and therefore integrates to zero over the entire region; that is to say, l_z is here globally, but not locally, a conserved quantity. If $\omega = \tilde{t}$, we find that

$$\sum_{\mu=0}^3 \frac{\partial J_\mu^{(\tilde{t})}}{\partial x^\mu}(t, x, y, z) = \psi^* \psi. \quad (22)$$

Hence, the so-called “dwell” time τ_D of the particle in a box B with the given input is the space-time integral of the density of creation of time over the box,

that is,

$$\tau_D = \iiint_B dt dx dy dz |\psi(t, x, y, z)|^2. \quad (23)$$

The latter result reproduces a formula given in Ref. [12] Eq. (2.2), Ref. [23] Eq. (2.67), and Ref. [24] Eq. (14). By the divergence theorem we can convert the volume integral to a surface integral, so that we have either

$$\tau_D^I = \left[\iiint_{\mathbb{R}^3} dx dy dz J_0^{(t)}(t, x, y, z) \right] \Big|_{t=t_1}^{t=t_2}, \text{ or} \quad (24a)$$

$$\tau_D^{II} = \left[\iiint_{\mathbb{R}^3} dt dx dy J_3^{(t)}(t, x, y, z) \right] \Big|_{z=z_1}^{z=z_2}. \quad (24b)$$

Hence if we have a boundary problem of Type I, such that $\psi(t, x, y, z)$ is zero on the spatial walls, and ψ has the usual conserved unit norm on the $t=\text{constant}$ walls, we find, with Eq. (20a)

$$\tau_D^I = t_2 - t_1. \quad (25)$$

If we have a boundary value problem of Type II—we will discuss later how to normalize ψ in that case—so that $\psi(t, x, y, z)$ tends to zero as t, x, y become large, and using Eq. (20b)

$$\begin{aligned} \tau_D^{II} &= \left[\frac{\hbar}{2im} \iint_{\mathbb{R}^3} dt dx dy \left(\psi(t, x, y, z)^* t \frac{\partial \psi}{\partial z}(t, x, y, z) \right. \right. \\ &\quad \left. \left. - \frac{\partial \psi^*}{\partial z}(t, x, y, z) t \psi(t, x, y, z) \right) \right] \Big|_{z=z_1}^{z=z_2}. \end{aligned} \quad (26)$$

But, given that we compute $\Psi(t, x, y, z)$ from $\psi(t, x, y, z)$ by Eq. (9), and that I_2 is the 2×2 unit matrix, then the operator tI_2 is the time operator in the z -evolution formalism, and we have, in the notation of Eq. (15),

$$\tau_D^{II} = (\Psi(z); (tI_2)\Psi(z)) \Big|_{z=z_1}^{z=z_2}. \quad (27)$$

The above results suggest that for a pseudo-Hermitean operator W in the space of Ψ -solutions, and for a boundary value problem of Type II, we should define the expectation value $\langle W \rangle_{\Psi(z)}$ of W in the state $\Psi(t, x, y, z)$ at a chosen z as

$$\langle W \rangle_{\Psi(z)} = (\Psi(z); W\Psi(z)), \quad (28)$$

as was proposed earlier in this section. The value $\langle W \rangle_{\Psi(z)}$ therefore (in Type II problems) specifies the average net flow of W across the given $z=\text{constant}$ surface. The difference of the expectation values of W computed at $z = z_2$ and $z = z_1$ is therefore the net flow of W out of the box, in other words is, on average, the total amount of W “created” by the system in the box.

We want now to define input and output on the spatial walls of the box. We define a complete, orthonormal basis $\phi_{(k_t, k_x, k_y)}(t, x, y)$ for all $(t, x, y) \in \mathbb{R}^3$ as follows:

$$\phi_{(k_t, k_x, k_y)}(t, x, y) = (2\pi)^{-3/2} \exp(-ik_t t + ik_x x + ik_y y), \quad (29)$$

where k_t , k_x , and k_y each range independently from $-\infty$ to $+\infty$. Although the physical dimension of k_t differs from that of k_x and k_y , it is convenient to use three-vector notation $\mathbf{k} = (k_t, k_x, k_y)$ and call the three-volume element $d^3k = dk_t dk_x dk_y$. The negative sign before k_t in the exponent in Eq. (29) is chosen so that positive k_t corresponds to positive energy; the conjugate momentum to t is $p_t \leftrightarrow (\hbar/i)\partial/\partial t \leftrightarrow -\hbar k_t$.

In an expansion of a wave function $\Psi(t, x, y, z)$ in the above basis functions, we will encounter certain quantities repeatedly, so we now define simplified notation for them: Let ζ take either value F or B , which stand for forward and backward motion along z , respectively. We also take

$$\sigma(\zeta) = \begin{cases} +1 & \text{if } \zeta = F, \\ -1 & \text{if } \zeta = B. \end{cases} \quad (30)$$

If $(2mk_t/\hbar) > (k_x^2 + k_y^2)$ (called an open channel), we define

$$k_z(\mathbf{k}) = [2mk_t/\hbar - k_x^2 - k_y^2]^{1/2}, \quad (31)$$

and if $(2mk_t/\hbar) < (k_x^2 + k_y^2)$ (called a closed channel), we define

$$\kappa_z(\mathbf{k}) = [-2mk_t/\hbar + k_x^2 + k_y^2]^{1/2}. \quad (32)$$

We shall normally just use k_z and κ_z without explicitly citing their arguments, except that primed, double primed, and triple primed arguments will be denoted, respectively, by k'_z , k''_z , and k'''_z , and similarly for κ_z .

Let a wave function have the expansion in basis functions

$$\Psi(t, x, y, z) = \iiint_{\mathbb{R}^3} d^3k \sum_{\zeta=B}^F f^\zeta(\mathbf{k}) \phi_\mathbf{k}(t, x, y) X^\zeta(\mathbf{k}; z), \quad (33)$$

where the $f^\zeta(\mathbf{k})$ are the expansion amplitudes, and where the $X^\zeta(\mathbf{k}; z)$ are normalized solutions for forward or backward motion along z , which we construct as follows: Substituting Eq. (33) into Eq. (10), we find that

$$\frac{1}{i} \frac{dX^\zeta}{dz}(\mathbf{k}; z) = H_{\text{sev}}(\mathbf{k}; z) X^\zeta(\mathbf{k}; z), \quad (34)$$

where, for V a function of z alone,

$$H_{\text{sev}}(\mathbf{k}; z) = \begin{bmatrix} 0 & 2mi/\hbar^2 \\ (\hbar^2/2mi)[2mk_t/\hbar - k_x^2 - k_y^2 - 2mV(z)/\hbar^2] & 0 \end{bmatrix}. \quad (35)$$

When $V(z) \equiv 0$, and for open channels, we obtain the solutions

$$X^\zeta(\mathbf{k}; z) = \begin{bmatrix} [m/(\hbar k_z)]^{1/2} \exp[\sigma(\zeta)i k_z z] \\ -\sigma(\zeta)(i/2)(\hbar^3 k_z/m)^{1/2} \exp[\sigma(\zeta)i k_z z] \end{bmatrix}; \quad (36)$$

the corresponding inner products are independent of z :

$$\hbar^{-1} X^{\zeta'}(\mathbf{k}; z)^\dagger M X^\zeta(\mathbf{k}; z) = \delta^{\zeta' \zeta} \sigma(\zeta). \quad (37)$$

Note, however, that these solutions do not satisfy the Cauchy inequality, in that $|\hbar^{-1} X^\zeta(\mathbf{k}')^\dagger M X^\zeta(\mathbf{k})| = (1/2)(\sqrt{k'_z/k_z} + \sqrt{k_z/k'_z})$, which is greater than 1 unless $k'_z = k_z$. For closed channels the solutions are

$$X^\zeta(\mathbf{k}; z) = \begin{bmatrix} [m/(\hbar\kappa_z)]^{1/2} \exp[-\sigma(\zeta)(i\pi/4 + \kappa_z z)] \\ \sigma(\zeta)(1/2)(\hbar^3 \kappa_z/m)^{1/2} \exp[-\sigma(\zeta)(i\pi/4 + \kappa_z z)] \end{bmatrix}; \quad (38)$$

the inner products take the z -independent forms

$$\hbar^{-1} X^{\zeta'}(\mathbf{k}; z)^\dagger M X^\zeta(\mathbf{k}; z) = \delta^{\zeta' F} \delta^{B\zeta} + \delta^{\zeta' B} \delta^{F\zeta}. \quad (39)$$

In general, the properties that distinguish between the four types of state of motion of a particle, that is open- versus closed-channel type, and F versus B type, depend on the local behavior of the state vector in wavenumber space (k_t, k_x, k_y) . The corresponding position (t, x, y) space forms of these properties are nonlocal. As mentioned in Section 5, these properties are likely to complicate an attempt to make a physical interpretation, in the context of the present formalism, of measurements at a given z of local properties in position t , x , or y . This is in contrast to standard quantum mechanics with t as the evolution coordinate, where there is only one type of state in x, y, z : F -type and open channel.

We note that the intermediate free-particle case $2mk_t/\hbar = k_x^2 + k_y^2$ gives rise to a “ghost” state, in that the reduced Hamiltonian on the rhs of Eq. (35) cannot be diagonalized by a similarity transformation. In this regard, the word “ghost” has undergone semantic drift since its use in the ’50’s—see Nagy [25], and [26], p. 14 for the former definition, and Kaku [27], p. 62, for the latter-day variant; wherein a state of negative norm is called a “ghost”. The recent usage is inappropriate here as states of negative norm are indispensable and ordinary, so I shall follow the earlier usage, which is motivated by the definition of the minimal polynomial of a finite-dimensional, square, complex matrix—see MacLane and Birkhoff [28], Ch. IX.6: Let L be a pseudo-Hermitean operator such that there exists a (real or nonreal) eigenvalue λ of L , an integer $n \geq 2$, and a state $X_{\lambda n}$ so that the state $(L - \lambda)^{n-1} X_{\lambda n}$ is not the zero state and is an eigenstate in that $(L - \lambda)^n X_{\lambda n} = 0$, then $X_{\lambda n}$ will be called a ghost state of L of Type n associated with the eigenvalue λ . We presume that, for any given L , and for each of its eigenvalues λ , there is a bounded number—possibly zero—of types of ghosts associated with it. The ghost states associated with fixed L and λ , and of different types n and m , are linearly independent of each other and of associated eigenstates; the direct sum of all the eigenstates and of all the corresponding linearly independent ghost states is a complete set of states in the overall space.

Continuing with the zero-potential-energy, intermediate-case solutions, we note that the symbols F and B are not useful. We take the solutions $X^\alpha(\hbar(k_x^2 +$

$k_y^2)/(2m), k_x, k_y; z)$ where $\alpha = 1, 2$, as follows:

$$X^1(\hbar(k_x^2 + k_y^2)/(2m), k_x, k_y; z) = \begin{bmatrix} [m\rho/\hbar]^{1/2} \\ 0 \end{bmatrix}, \quad (40a)$$

$$X^2(\hbar(k_x^2 + k_y^2)/(2m), k_x, k_y; z) = \begin{bmatrix} [m/(\rho\hbar)]^{1/2} 2iz \\ -i[\hbar^3/(m\rho)]^{1/2} \end{bmatrix}, \quad (40b)$$

where ρ is an arbitrary positive number of dimension *length* introduced to make the components dimensionally consistent with Eqs. (36) and (38). The inner products are also z -independent:

$$\begin{aligned} \hbar^{-1} X^{\alpha'}(\hbar(k_x^2 + k_y^2)/(2m), k_x, k_y; z)^\dagger M X^\alpha(\hbar(k_x^2 + k_y^2)/(2m), k_x, k_y; z) \\ = \begin{cases} 0, & \text{if } \alpha' = \alpha, \\ +1, & \text{if } \alpha' \neq \alpha. \end{cases} \end{aligned} \quad (41)$$

Physically, the states in the intermediate case propagate parallel to any plane $z=\text{constant}$, that is, neither forward nor backward along z . Note that the solution Eq. (40a) is, and that of Eq. (40b) is not, an eigenstate with eigenvalue zero of the reduced Hamiltonian on the rhs of Eq. (35); in fact, the X^2 is a ghost state of Type 2 for any choice of k_x, k_y and z .

We next compute the inner product at each z of two free-particle wave functions $\Psi(t, x, y, z)$ and $\Phi(t, x, y, z)$, when they have expansion amplitudes $f^\zeta(\mathbf{k})$ and $g^\zeta(\mathbf{k})$, respectively. It is convenient to divide \mathbf{k} -space into domains for open and closed channels:

$$\iiint_{\text{open}} d^3k = \iint_{\mathbb{R}^2} dk_x dk_y \int_{\hbar(k_x^2 + k_y^2)/2m}^{\infty} dk_t, \quad (42a)$$

$$\iiint_{\text{closed}} d^3k = \iint_{\mathbb{R}^2} dk_x dk_y \int_{-\infty}^{\hbar(k_x^2 + k_y^2)/2m} dk_t, \quad (42b)$$

$$\iiint_{\mathbb{R}^3} d^3k = \iiint_{\text{open}} d^3k + \iiint_{\text{closed}} d^3k. \quad (42c)$$

The inner product of Ψ and Φ is z -independent, and takes the form

$$\begin{aligned} (\Psi(z); \Phi(z)) = & \iiint_{\text{open}} d^3k \sum_{\zeta=B}^F \sigma(\zeta) f^\zeta(\mathbf{k})^* g^\zeta(\mathbf{k}) \\ & + \iiint_{\text{closed}} d^3k [f^F(\mathbf{k})^* g^B(\mathbf{k}) + f^B(\mathbf{k})^* g^F(\mathbf{k})]. \end{aligned} \quad (43)$$

Note that the subspace generated by “ F ” open-channel states has a positive definite norm, while the space of “ B ” open-channel states has a negative definite norm; both of these subspaces therefore comprise a Hilbert space. In the scattering phenomena analysed in Section 3 we shall discover that the open-channel sub-matrix of the S -matrix is unitary, and preserves the inner product

of two vectors belonging to a direct sum of these Hilbert spaces referring to different z -planes, assembled so that the sign of the inner product and metric are reversed in the second subspace component—hence there is a positive definite metric overall. The “ F ” and “ B ” Hilbert spaces on any z =constant plane are of limited utility, as most linear operators encountered in the space of states do not map such a Hilbert space into itself, but generate superpositions of open- and closed-channel states.

The question of normalizing the space-evolving wave functions can now be addressed: If the potential $V(t, x, y, z) \neq 0$ in, and only in, the interior of the box \mathcal{B}_2 , a solution $\Psi(t, x, y, z)$ of Eq. (10) can be expressed in an expansion of the type Eq. (33), belonging to potential-free regions, in the neighborhood of both $z = z_1$ and $z = z_2$, but with different expansion amplitudes at each end of the interval. We first define the basis functions

$$\Xi^\zeta(\mathbf{k}; t, x, y, z) = (2\pi)^{-3/2} \exp(-ik_t t + ik_x x + ik_y y) X^\zeta(\mathbf{k}; z). \quad (44)$$

We assume here and unless otherwise stated that there is no closed-channel input, and adopt the following conventions:

$$\begin{aligned} \Psi(t, x, y, z_1) &= \iiint_{\text{open}} d^3 k f_{\text{in}}^F(\mathbf{k}) \Xi^F(\mathbf{k}; t, x, y, z_1) \\ &\quad + \iiint_{\mathbb{R}^3} d^3 k f_{\text{out}}^B(\mathbf{k}) \Xi^B(\mathbf{k}; t, x, y, z_1), \end{aligned} \quad (45a)$$

$$\begin{aligned} \Psi(t, x, y, z_2) &= \iiint_{\text{open}} d^3 k f_{\text{in}}^B(\mathbf{k}) \Xi^B(\mathbf{k}; t, x, y, z_2) \\ &\quad + \iiint_{\mathbb{R}^3} d^3 k f_{\text{out}}^F(\mathbf{k}) \Xi^F(\mathbf{k}; t, x, y, z_2), \end{aligned} \quad (45b)$$

Since the flow of particle presence is conserved, the norms of $\Psi(t, x, y, z_1)$ and $\Psi(t, x, y, z_2)$ are equal:

$$\langle \tilde{1} \rangle_{\Psi(z_2)} = \langle \tilde{1} \rangle_{\Psi(z_1)}. \quad (46)$$

Note that at $z = z_1$, the forward and backward flowing parts of the wave function correspond to input and output, respectively, with the opposite association at $z = z_2$. Note also that for a time-dependent potential energy there will be scattering from open-channel input into both open- and closed-channel output, which circumstance is accounted for in Eq. (45). We now define a normalized, Type II wave function as one for which the input amplitude function is normalized to one, that is,

$$\begin{aligned} 1 &= \iiint_{\text{open}} d^3 k [|f_{\text{in}}^F(\mathbf{k})|^2 + |f_{\text{in}}^B(\mathbf{k})|^2] \\ &= \iiint_{\text{open}} d^3 k [|f_{\text{out}}^F(\mathbf{k})|^2 + |f_{\text{out}}^B(\mathbf{k})|^2], \end{aligned} \quad (47)$$

where the second equation follows from Eqs. (43), (45), and (46). Note that there is no contribution to the output normalization from closed-channel amplitudes.

We conclude the section by developing a formula for the expectation value of the operator $\check{t}I_2$ in terms of the wave-number space expansion amplitudes $f^\zeta(\mathbf{k})$. Let $\Psi(t, x, y, z)$ be as in Eq. (33). Then we have

$$\begin{aligned}\langle \check{t}I_2 \rangle_{\Psi(z)} &= \hbar^{-1} \iiint_{\mathbb{R}^3} dt dx dy \iiint_{\mathbb{R}^3} d^3 k \sum_{\zeta=B}^F \Psi(t, x, y, z)^\dagger M \\ &\quad \times f^\zeta(\mathbf{k}) (2\pi)^{-3/2} t \exp[-ik_t t + ik_x x + ik_y y] X^\zeta(\mathbf{k}; z).\end{aligned}\quad (48)$$

Replacing $t \exp[-ik_t t]$ by $i(\partial/\partial k_t) \exp[-ik_t t]$ and integrating by parts on k_t , we find that

$$\begin{aligned}\langle \check{t}I_2 \rangle_{\Psi(z)} &= \hbar^{-1} \iiint_{\mathbb{R}^3} dt dx dy \iiint_{\mathbb{R}^3} d^3 k \sum_{\zeta=B}^F \Psi(t, x, y, z)^\dagger M \\ &\quad \times (2\pi)^{-3/2} \exp[-ik_t t + ik_x x + ik_y y] \frac{1}{i} \frac{\partial}{\partial k_t} [f^\zeta(\mathbf{k}) X^\zeta(\mathbf{k}; z)].\end{aligned}\quad (49)$$

Analogous to spatial position operators in momentum space, the operator for t transforms into $-i\partial/\partial k_t$, the sign difference being a result of the negative sign in the exponent in Eq. (29). This result agrees with that in Ref. [29], Ch. 8, Eq. (286); see also [16], §8.

The evaluation of Eq. (49) is facilitated by the following formulas: for $\zeta = F$ and B and for $\zeta' = B$ and F , respectively, and for open channels,

$$\hbar^{-1} X^\zeta(\mathbf{k}; z)^\dagger M \frac{1}{i} \frac{\partial X^\zeta}{\partial k_t}(\mathbf{k}; z) = \frac{mz}{\hbar k_z}, \quad (50a)$$

$$\hbar^{-1} X^\zeta(\mathbf{k}; z)^\dagger M \frac{1}{i} \frac{\partial X^{\zeta'}}{\partial k_t}(\mathbf{k}; z) = \sigma(\zeta) \frac{im}{2\hbar k_z^2} \exp(-\sigma(\zeta) 2ik_z z), \quad (50b)$$

while for closed channels

$$\hbar^{-1} X^\zeta(\mathbf{k}; z)^\dagger M \frac{1}{i} \frac{\partial X^\zeta}{\partial k_t}(\mathbf{k}; z) = -\sigma(\zeta) \frac{m}{2\hbar \kappa_z^2} \exp(-\sigma(\zeta) 2\kappa_z z), \quad (51a)$$

$$\hbar^{-1} X^\zeta(\mathbf{k}; z)^\dagger M \frac{1}{i} \frac{\partial X^{\zeta'}}{\partial k_t}(\mathbf{k}; z) = \sigma(\zeta) \frac{imz}{\hbar \kappa_z}. \quad (51b)$$

If we carry out the differentiations in the integrand of Eq. (49), we find that

$$\begin{aligned}
\langle \tilde{t}I_2 \rangle_{\Psi(z)} &= \iiint_{\text{open}} d^3k \left[\sum_{\zeta=B}^F \left(\sigma(\zeta) f^\zeta(\mathbf{k})^* \frac{1}{i} \frac{\partial f^\zeta}{\partial k_t}(\mathbf{k}) \right) \right. \\
&\quad - \frac{im}{2\hbar k_z^2} \exp(+2ik_z z) f^B(\mathbf{k})^* f^F(\mathbf{k}) \\
&\quad + \frac{im}{2\hbar k_z^2} \exp(-2ik_z z) f^F(\mathbf{k})^* f^B(\mathbf{k}) \\
&\quad \left. + \frac{mz}{\hbar k_z} (|f^F(\mathbf{k})|^2 + |f^B(\mathbf{k})|^2) \right] + \iiint_{\text{closed}} d^3k \\
&\quad \times \left[f^B(\mathbf{k})^* \frac{1}{i} \frac{\partial f^F}{\partial k_t}(\mathbf{k}) + f^F(\mathbf{k})^* \frac{1}{i} \frac{\partial f^B}{\partial k_t}(\mathbf{k}) \right. \\
&\quad - \frac{m}{2\hbar \kappa_z^2} \exp(-2\kappa_z z) |f^F(\mathbf{k})|^2 + \frac{m}{2\hbar \kappa_z^2} \exp(+2\kappa_z z) |f^B(\mathbf{k})|^2 \\
&\quad \left. - \frac{imz}{\hbar \kappa_z} f^B(\mathbf{k})^* f^F(\mathbf{k}) + \frac{imz}{\hbar \kappa_z} f^F(\mathbf{k})^* f^B(\mathbf{k}) \right]. \tag{52}
\end{aligned}$$

Due to the denominators involving k_z^2 or κ_z^2 in the above, convergence of the integrals requires that the $f^\zeta(\mathbf{k})$ approach zero sufficiently rapidly as \mathbf{k} approaches the boundary between open and closed channels.

3 Scattering; dwell and delay times

In this section, we shall presume the presence of a generic potential energy distribution $V(t, x, y, z)$, such that its support is contained within the box \mathcal{B}_2 . The potential energy gives rise to scattering of the (we presume, purely open-channel) input signals, such that reflected and transmitted waves across the spectrum of \mathbf{k} , including both open and closed channels, will comprise the output signal from the box. We now assume that our prescription for specifying the input yields necessary and sufficient information such that a solution to the Schrödinger equation within the box exists, satisfies the input boundary conditions, and is unique. Accordingly, the output is determined by the input, and this association must be linear in view of the linearity of the Schrödinger equation. The linear operator specifying this association consists of reflection and transmission coefficients, which can be assembled into an S -matrix, which—as we shall verify—has a submatrix, referring to purely open-channel output as well as input, that is unitary.

We presume that the Schrödinger equation has been solved for all open-

channel inputs, and express the output linearly in terms of the input as follows:

$$\begin{aligned} f_{\text{out}}^B(\mathbf{k}) &= \iiint_{\text{open}} d^3 k' \\ &\times [R^{BF}(\mathbf{k}; \mathbf{k}') f_{\text{in}}^F(\mathbf{k}') \\ &+ T^{BB}(\mathbf{k}; \mathbf{k}') f_{\text{in}}^B(\mathbf{k}')], \end{aligned} \quad (53)$$

$$\begin{aligned} f_{\text{out}}^F(\mathbf{k}) &= \iiint_{\text{open}} d^3 k' \\ &\left[T^{FF}(\mathbf{k}; \mathbf{k}') f_{\text{in}}^F(\mathbf{k}') \right. \\ &\left. + R^{FB}(\mathbf{k}; \mathbf{k}') f_{\text{in}}^B(\mathbf{k}') \right]. \end{aligned} \quad (54)$$

The functions T^{FF} , R^{FB} , R^{BF} , and T^{BB} are reflection and transmission coefficients, where the input-to-output superscripts are to be read from right to left. In Eqs. (53) and (54), consistent with Eqs. (45a) and (45b), the reflection and transmission coefficients are defined for the output parameter k_t having either an open- or a closed-channel value.

For later convenience, we define

$$I^{\text{open}}(\mathbf{k}' - \mathbf{k}'') = \delta^{\text{open}}(k'_t - k''_t) \delta(k'_x - k''_x) \delta(k'_y - k''_y), \quad (55)$$

where $\delta^{\text{open}}(k'_t - k''_t)$ is defined only for both k'_t and k''_t corresponding to open channels.

Let us now substitute Eqs. (53) and (54) into Eq. (47). We obtain a quadratic expression in the input amplitudes f_{in}^ζ on both sides of the resulting equation. Since the these amplitude functions are arbitrary, the coefficients of the four quadratic terms must be equal. We infer that, for both k'_t and k''_t being of open-channel type,

$$\begin{aligned} &\iiint_{\text{open}} d^3 k \left[T^{FF}(\mathbf{k}; \mathbf{k}')^* T^{FF}(\mathbf{k}; \mathbf{k}'') \right. \\ &\left. + R^{BF}(\mathbf{k}; \mathbf{k}')^* R^{BF}(\mathbf{k}; \mathbf{k}'') \right] \\ &= I^{\text{open}}(\mathbf{k}' - \mathbf{k}''), \end{aligned} \quad (56)$$

$$\begin{aligned} &\iiint_{\text{open}} d^3 k \left[R^{FB}(\mathbf{k}; \mathbf{k}')^* R^{FB}(\mathbf{k}; \mathbf{k}'') \right. \\ &\left. + T^{BB}(\mathbf{k}; \mathbf{k}')^* T^{BB}(\mathbf{k}; \mathbf{k}'') \right] \\ &= I^{\text{open}}(\mathbf{k}' - \mathbf{k}''), \end{aligned} \quad (57)$$

$$\begin{aligned} &\iiint_{\text{open}} d^3 k \left[R^{FB}(\mathbf{k}; \mathbf{k}')^* T^{FF}(\mathbf{k}; \mathbf{k}'') \right. \\ &\left. + T^{BB}(\mathbf{k}; \mathbf{k}')^* R^{BF}(\mathbf{k}; \mathbf{k}'') \right] = 0, \end{aligned} \quad (58)$$

$$\begin{aligned} & \iiint_{\text{open}} d^3 k \left[R^{BF}(\mathbf{k}; \mathbf{k}')^* T^{BB}(\mathbf{k}; \mathbf{k}'') \right. \\ & \left. + T^{FF}(\mathbf{k}; \mathbf{k}')^* R^{FB}(\mathbf{k}; \mathbf{k}'') \right] = 0. \end{aligned} \quad (59)$$

Let us now make up an S -matrix and its transpose conjugate S^\dagger from the reflection and transmission matrices. In the following, the unprimed index k_t ranges over all real values, while k'_t and k''_t range over open-channel values only:

$$\begin{aligned} S(\mathbf{k}; \mathbf{k}'') \\ = \begin{bmatrix} T^{FF}(\mathbf{k}; \mathbf{k}'') & R^{FB}(\mathbf{k}; \mathbf{k}'') \\ R^{BF}(\mathbf{k}; \mathbf{k}'') & T^{BB}(\mathbf{k}; \mathbf{k}'') \end{bmatrix}, \end{aligned} \quad (60)$$

$$\begin{aligned} S^\dagger(\mathbf{k}'; \mathbf{k}) \\ = \begin{bmatrix} T^{FF}(\mathbf{k}; \mathbf{k}')^* & R^{BF}(\mathbf{k}; \mathbf{k}')^* \\ R^{FB}(\mathbf{k}; \mathbf{k}')^* & T^{BB}(\mathbf{k}; \mathbf{k}')^* \end{bmatrix}. \end{aligned} \quad (61)$$

It is convenient to define two submatrices of S , the open-channel part S_o and the closed-channel part S_c as follows:

$$S_o(\mathbf{k}; \mathbf{k}') = S(\mathbf{k}; \mathbf{k}'), \quad \text{for all } k_t > (\hbar/2m)(k_x^2 + k_y^2), \quad (62a)$$

$$S_c(\mathbf{k}; \mathbf{k}') = S(\mathbf{k}; \mathbf{k}'), \quad \text{for all } k_t < (\hbar/2m)(k_x^2 + k_y^2). \quad (62b)$$

Then S_o is unitary on the left as a result of Eqs. (56)–(59):

$$\begin{aligned} (S_o^\dagger S_o)(\mathbf{k}'; \mathbf{k}'') \\ = \iiint_{\text{open}} d^3 k [S_o^\dagger(\mathbf{k}'; \mathbf{k}) S_o(\mathbf{k}; \mathbf{k}'')] \\ = I_2 \otimes I^{\text{open}}(\mathbf{k}' - \mathbf{k}''). \end{aligned} \quad (63)$$

One expects that S_o is also unitary on the right,

$$(S_o S_o^\dagger)(\mathbf{k}'; \mathbf{k}'') = I_2 \otimes I^{\text{open}}(\mathbf{k}' - \mathbf{k}''). \quad (64)$$

We now reduce the formulas for the expectation values of the operator $\tilde{t}I_2$ at $z = z_1, z_2$, using Eqs. (45), (52), (53), and (54), and then establish a relatively simple form for the difference of the two values. We assume that the input amplitudes $f_{\text{in}}^\zeta(\mathbf{k})$ and the output state values of the S -matrix elements go to zero at the open/closed-channel threshold so that the following integrals converge. We have first

$$\begin{aligned} \langle \tilde{t}I_2 \rangle_{\Psi(z_1)} &= \iiint_{\text{open}} d^3 k f_{\text{in}}^F(\mathbf{k})^* \frac{1}{i} \frac{\partial f_{\text{in}}^F}{\partial k_t}(\mathbf{k}) \\ &+ \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \sum_{\zeta, \zeta'} \\ &\times f_{\text{in}}^\zeta(\mathbf{k})^* A^{\zeta \zeta'}(\mathbf{k}; \mathbf{k}'; z_1) f_{\text{in}}^{\zeta'}(\mathbf{k}'). \end{aligned} \quad (65)$$

The matrix of coefficients is as follows:

$$\begin{aligned}
A^{FF}(\mathbf{k}; \mathbf{k}'; z_1) &= \frac{mz_1}{\hbar k_z} I^{\text{open}}(\mathbf{k} - \mathbf{k}') \\
&+ \frac{im}{2\hbar k_z^2} \exp(-2ik_z z_1) R^{BF}(\mathbf{k}; \mathbf{k}') \\
&- R^{BF}(\mathbf{k}'; \mathbf{k})^* \frac{im}{2\hbar k_z'^2} \exp(+2ik_z' z_1) \\
&+ \iiint_{\text{open}} d^3 k'' R^{BF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \left[\frac{mz_1}{\hbar k_z''} - \frac{1}{i} \frac{\partial}{\partial k_t''} \right] R^{BF}(\mathbf{k}''; \mathbf{k}') \\
&+ \iiint_{\text{closed}} d^3 k'' R^{BF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \frac{m}{2\hbar \kappa_z''^2} \exp(2\kappa_z'' z_1) R^{BF}(\mathbf{k}''; \mathbf{k}');
\end{aligned} \tag{66}$$

$$\begin{aligned}
A^{FB}(\mathbf{k}; \mathbf{k}'; z_1) &= \frac{im}{2\hbar k_z^2} \exp(-2ik_z z_1) T^{BB}(\mathbf{k}; \mathbf{k}') \\
&+ \iiint_{\text{open}} d^3 k'' R^{BF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \left[\frac{mz_1}{\hbar k_z''} - \frac{1}{i} \frac{\partial}{\partial k_t''} \right] T^{BB}(\mathbf{k}''; \mathbf{k}') \\
&+ \iiint_{\text{closed}} d^3 k'' R^{BF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \frac{m}{2\hbar \kappa_z''^2} \exp(2\kappa_z'' z_1) T^{BB}(\mathbf{k}''; \mathbf{k}');
\end{aligned} \tag{67}$$

$$\begin{aligned}
A^{BF}(\mathbf{k}; \mathbf{k}'; z_1) &= -T^{BB}(\mathbf{k}'; \mathbf{k})^* \frac{im}{2\hbar k_z'^2} \exp(2ik_z' z_1) \\
&+ \iiint_{\text{open}} d^3 k'' T^{BB}(\mathbf{k}''; \mathbf{k})^* \\
&\times \left[\frac{mz_1}{\hbar k_z''} - \frac{1}{i} \frac{\partial}{\partial k_t''} \right] R^{BF}(\mathbf{k}''; \mathbf{k}') \\
&+ \iiint_{\text{closed}} d^3 k'' T^{BB}(\mathbf{k}''; \mathbf{k})^* \\
&\times \frac{m}{2\hbar \kappa_z''^2} \exp(2\kappa_z'' z_1) R^{BF}(\mathbf{k}''; \mathbf{k}');
\end{aligned} \tag{68}$$

$$\begin{aligned}
A^{BB}(\mathbf{k}; \mathbf{k}'; z_1) &= \iiint_{\text{open}} d^3 k'' T^{BB}(\mathbf{k}''; \mathbf{k})^* \\
&\times \left[\frac{mz_1}{\hbar k_z''} - \frac{1}{i} \frac{\partial}{\partial k_t''} \right] T^{BB}(\mathbf{k}''; \mathbf{k}') \\
&+ \iiint_{\text{closed}} d^3 k'' T^{BB}(\mathbf{k}''; \mathbf{k})^* \\
&\times \frac{m}{2\hbar\kappa_z''^2} \exp(2\kappa_z'' z_1) T^{BB}(\mathbf{k}''; \mathbf{k}').
\end{aligned} \tag{69}$$

At $z = z_2$ we have

$$\begin{aligned}
\langle \tilde{t}I_2 \rangle_{\Psi(z_2)} &= - \iiint_{\text{open}} d^3 k f_{\text{in}}^B(\mathbf{k})^* \frac{1}{i} \frac{\partial f_{\text{in}}^B}{\partial k_t}(\mathbf{k}) \\
&+ \iint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \sum_{\zeta, \zeta'} \\
&\times f_{\text{in}}^\zeta(\mathbf{k})^* C^{\zeta\zeta'}(\mathbf{k}; \mathbf{k}'; z_2) f_{\text{in}}^{\zeta'}(\mathbf{k}').
\end{aligned} \tag{70}$$

In the above, the coefficient matrices are

$$\begin{aligned}
C^{FF}(\mathbf{k}; \mathbf{k}'; z_2) &= \iiint_{\text{open}} d^3 k'' T^{FF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \left[\frac{mz_2}{\hbar k_z''} + \frac{1}{i} \frac{\partial}{\partial k_t''} \right] T^{FF}(\mathbf{k}''; \mathbf{k}') \\
&- \iiint_{\text{closed}} d^3 k'' T^{FF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \frac{m}{2\hbar\kappa_z''^2} \exp(-2\kappa_z'' z_2) T^{FF}(\mathbf{k}''; \mathbf{k}');
\end{aligned} \tag{71}$$

$$\begin{aligned}
C^{FB}(\mathbf{k}; \mathbf{k}'; z_2) &= T^{FF}(\mathbf{k}'; \mathbf{k})^* \frac{im}{2\hbar k_z'^2} \exp(-2ik_z' z_2) \\
&+ \iiint_{\text{open}} d^3 k'' T^{FF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \left[\frac{mz_2}{\hbar k_z''} + \frac{1}{i} \frac{\partial}{\partial k_t''} \right] R^{FB}(\mathbf{k}''; \mathbf{k}) \\
&- \iiint_{\text{closed}} d^3 k'' T^{FF}(\mathbf{k}''; \mathbf{k})^* \\
&\times \frac{m}{2\hbar\kappa_z''^2} \exp(-2\kappa_z'' z_2) R^{FB}(\mathbf{k}''; \mathbf{k}');
\end{aligned} \tag{72}$$

$$\begin{aligned}
C^{BF}(\mathbf{k}; \mathbf{k}'; z_2) &= -\frac{im}{2\hbar k_z^2} \exp(2ik_z z_2) T^{FF}(\mathbf{k}; \mathbf{k}') \\
&\quad + \iiint_{\text{open}} d^3 k'' R^{FB}(\mathbf{k}''; \mathbf{k})^* \\
&\quad \times \left[\frac{mz_2}{\hbar k_z''} + \frac{1}{i} \frac{\partial}{\partial k_t''} \right] T^{FF}(\mathbf{k}''; \mathbf{k}') \\
&\quad - \iiint_{\text{closed}} d^3 k'' R^{FB}(\mathbf{k}''; \mathbf{k})^* \\
&\quad \times \frac{m}{2\hbar \kappa_z''^2} \exp(-2\kappa_z'' z_2) T^{FF}(\mathbf{k}''; \mathbf{k}'); \tag{73}
\end{aligned}$$

$$\begin{aligned}
C^{BB}(\mathbf{k}; \mathbf{k}'; z_2) &= \frac{mz_2}{\hbar k_z} I^{\text{open}}(\mathbf{k} - \mathbf{k}') \\
&\quad - \frac{im}{2\hbar k_z^2} \exp(2ik_z z_2) R^{FB}(\mathbf{k}; \mathbf{k}') \\
&\quad + R^{FB}(\mathbf{k}'; \mathbf{k})^* \frac{im}{2\hbar k_z'} \exp(-2ik_z' z_2) \\
&\quad + \iiint_{\text{open}} d^3 k'' R^{FB}(\mathbf{k}''; \mathbf{k})^* \\
&\quad \times \left[\frac{mz_2}{\hbar k_z''} + \frac{1}{i} \frac{\partial}{\partial k_t''} \right] R^{FB}(\mathbf{k}''; \mathbf{k}') \\
&\quad - \iiint_{\text{closed}} d^3 k'' R^{FB}(\mathbf{k}''; \mathbf{k}')^* \\
&\quad \times \frac{m}{2\hbar \kappa_z''^2} \exp(-2\kappa_z'' z_2) R^{FB}(\mathbf{k}''; \mathbf{k}'). \tag{74}
\end{aligned}$$

The difference of the two expectation values takes the form

$$\begin{aligned}
\langle \tilde{t}I_2 \rangle_{\Psi(z_2)} - \langle \tilde{t}I_2 \rangle_{\Psi(z_1)} &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \\
&\quad \times \sum_{\zeta, \zeta'} f_{\text{in}}^\zeta(\mathbf{k})^* D^{\zeta \zeta'}(\mathbf{k}; \mathbf{k}'; z_1; z_2) f_{\text{in}}^{\zeta'}(\mathbf{k}'). \tag{75}
\end{aligned}$$

We break the D -matrices into constituents:

$$D = D_1 + M D_2 S_o + S_o^\dagger D_2^\dagger M + S_o^\dagger D_3 S_o + S_c^\dagger D_4 S_c, \tag{76}$$

where

$$D_1 = I^{\text{open}}(\mathbf{k} - \mathbf{k}') \otimes \text{diag} \left(-\frac{1}{i} \frac{\partial}{\partial k_t'} - \frac{mz_1}{\hbar k_z'}, -\frac{1}{i} \frac{\partial}{\partial k_t'} + \frac{mz_2}{\hbar k_z'} \right), \tag{77}$$

$$D_2 = \text{diag} \left(\frac{m}{2\hbar k_z^2} \exp(2ik_z z_2), -\frac{m}{2\hbar k_z^2} \exp(-2ik_z z_1) \right), \tag{78}$$

$$D_3 = \text{diag}\left(\frac{1}{i} \frac{\partial}{\partial k_t''} + \frac{mz_2}{\hbar k_z''}, \frac{1}{i} \frac{\partial}{\partial k_t''} - \frac{mz_1}{\hbar k_z''}\right) \quad (79)$$

$$D_4 = \text{diag}\left(-\frac{m}{2\hbar\kappa_z'^2} \exp(-2\kappa_z'' z_2), -\frac{m}{2\hbar\kappa_z'^2} \exp(2\kappa_z'' z_1)\right). \quad (80)$$

In Eqs. (79) and (80), the double primes indicate the dummy variables of integration implicit in the final two summands on the rhs of Eq. (76).

It is plausible that Eq. (75), given that the total input is normalized as in Eq. (47), provides a complete expression for the mean dwell time of the particle in the box, inasmuch as it is also an expression for the space-time integral over the box of the divergence of the flow vector density of time. We remark that if the potential energy is time-independent, then the S_o -matrix takes the form $S_o(\mathbf{k}''; \mathbf{k}') = \delta^{\text{open}}(\mathbf{k}_t'' - \mathbf{k}_t') \tilde{S}_o(\mathbf{k}_t'', \mathbf{k}_x'', \mathbf{k}_y''; \mathbf{k}_x', \mathbf{k}_y')$; one can now show that, due to the unitarity of S_o , the terms involving $-i\partial f_{\text{in}}^{\zeta}/\partial k_t'(\mathbf{k}')$ cancel out in the overall expression for the dwell time. This cancellation does not, as we shall see, occur for the individual delay times for transmission or reflection from a zone of time-independent interaction.

The average delay times that are measured in beam experiments for either transmission or reflection are not so fundamentally defined. We simplify the problem as follows: First, we assume that only one kind of input, that is F or but not B, is present. Second, we assume that the closed-channel contributions will be negligible in the measuring apparatus. Third, we neglect interference between the incoming signal and the outgoing signal in the case of reflection (hence, the contributions linear in the S -matrix are discarded). We now specify what remains after these simplifications.

In the first instance, let $f_{\text{in}}^B(\mathbf{k}) \equiv 0$, and let f_{in}^F be normalized as in Eq. (47). The net outgoing reflected and transmitted currents of particle presence are called $\mathcal{R}_{B \leftarrow F}^{\text{out}}(z_1)$ and $\mathcal{T}_{F \leftarrow F}^{\text{out}}(z_2)$, respectively, and take the values

$$\begin{aligned} \mathcal{R}_{B \leftarrow F}^{\text{out}}(z_1) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \iiint_{\text{open}} d^3 k'' [f_{\text{in}}^F(\mathbf{k})^* \\ &\times (-1) R^{BF}(\mathbf{k}''; \mathbf{k})^* R^{BF}(\mathbf{k}''; \mathbf{k}') f_{\text{in}}^F(\mathbf{k}')], \end{aligned} \quad (81a)$$

$$\begin{aligned} \mathcal{T}_{F \leftarrow F}^{\text{out}}(z_2) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \iiint_{\text{open}} d^3 k'' [f_{\text{in}}^F(\mathbf{k})^* \\ &\times T^{FF}(\mathbf{k}''; \mathbf{k})^* T^{FF}(\mathbf{k}''; \mathbf{k}') f_{\text{in}}^F(\mathbf{k}')]. \end{aligned} \quad (81b)$$

According to Eq. (56), we have

$$\mathcal{T}_{F \leftarrow F}^{\text{out}}(z_2) - \mathcal{R}_{B \leftarrow F}^{\text{out}}(z_1) = 1. \quad (82)$$

The mean currents of time at entry and upon reflection at z_1 , and upon transmission at z_2 , will be called, respectively, $\tau_F^{\text{in}}(z_1)$, $\tau_{B \leftarrow F}^{\text{out}}(z_1)$, and $\tau_{F \leftarrow F}^{\text{out}}(z_2)$, and can be inferred from Eqs. (66) (twice) and (71), subject to the three simplifica-

tions spelled out in the previous paragraph, as follows:

$$\tau_F^{\text{in}}(z_1) = \iiint_{\text{open}} d^3 k f_{\text{in}}^F(\mathbf{k})^* \left[\frac{1}{i} \frac{\partial}{\partial k_t} + \frac{mz_1}{\hbar k_z} \right] f_{\text{in}}^F(\mathbf{k}), \quad (83a)$$

$$\begin{aligned} \tau_{B \leftarrow F}^{\text{out}}(z_1) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \left\{ f_{\text{in}}^F(\mathbf{k})^* \iiint_{\text{open}} d^3 k'' R^{BF}(\mathbf{k}''; \mathbf{k})^* \right. \\ &\times \left. \left[-\frac{1}{i} \frac{\partial}{\partial k_t''} + \frac{mz_1}{\hbar k_z''} \right] R^{BF}(\mathbf{k}''; \mathbf{k}') \right\} f_{\text{in}}^F(\mathbf{k}'), \end{aligned} \quad (83b)$$

$$\begin{aligned} \tau_{F \leftarrow F}^{\text{out}}(z_2) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \left\{ f_{\text{in}}^F(\mathbf{k})^* \iiint_{\text{open}} d^3 k'' T^{FF}(\mathbf{k}''; \mathbf{k})^* \right. \\ &\times \left. \left[\frac{1}{i} \frac{\partial}{\partial k_t''} + \frac{mz_2}{\hbar k_z''} \right] T^{FF}(\mathbf{k}''; \mathbf{k}') \right\}. \end{aligned} \quad (83c)$$

In the second instance, let $f_{\text{in}}^F(\mathbf{k}) \equiv 0$, and let $f_{\text{in}}^B(\mathbf{k})$ be normalized as in Eq. (47). The net outgoing reflected and transmitted currents of particle presence are called $\mathcal{R}_{F \leftarrow B}^{\text{out}}(z_2)$ and $\mathcal{T}_{B \leftarrow B}^{\text{out}}(z_1)$, respectively, and take the values

$$\begin{aligned} \mathcal{R}_{F \leftarrow B}^{\text{out}}(z_2) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \iiint_{\text{open}} d^3 k'' [f_{\text{in}}^B(\mathbf{k})^* \\ &\times R^{FB}(\mathbf{k}''; \mathbf{k})^* R^{FB}(\mathbf{k}''; \mathbf{k}') f_{\text{in}}^B(\mathbf{k}')], \end{aligned} \quad (84a)$$

$$\begin{aligned} \mathcal{T}_{B \leftarrow B}^{\text{out}}(z_1) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \iiint_{\text{open}} d^3 k'' [f_{\text{in}}^B(\mathbf{k})^* T^{BB}(\mathbf{k}''; \mathbf{k})^* \\ &\times (-1) T^{BB}(\mathbf{k}''; \mathbf{k}') f_{\text{in}}^B(\mathbf{k}')]. \end{aligned} \quad (84b)$$

According to Eq. (57), we have

$$\mathcal{R}_{F \leftarrow B}^{\text{out}}(z_2) - \mathcal{T}_{B \leftarrow B}^{\text{out}}(z_1) = 1. \quad (85)$$

The net currents of time at z_2 upon entry and after reflection, and at z_1 after transmission, will be called, respectively, $\tau_B^{\text{in}}(z_2)$, $\tau_{F \leftarrow B}^{\text{out}}(z_2)$, and $\tau_{B \leftarrow B}^{\text{out}}(z_1)$, and can be inferred from Eqs. (74) (twice) and (69), subject to the three simplifications given previously, as follows:

$$\tau_B^{\text{in}}(z_2) = \iiint_{\text{open}} d^3 k f_{\text{in}}^B(\mathbf{k})^* \left[-\frac{1}{i} \frac{\partial}{\partial k_t} + \frac{mz_2}{\hbar k_z} \right] f_{\text{in}}^B(\mathbf{k}), \quad (86a)$$

$$\begin{aligned} \tau_{F \leftarrow B}^{\text{out}}(z_2) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \left\{ f_{\text{in}}^B(\mathbf{k})^* \iiint_{\text{open}} d^3 k'' R^{FB}(\mathbf{k}''; \mathbf{k})^* \right. \\ &\times \left. \left[\frac{1}{i} \frac{\partial}{\partial k_t''} + \frac{mz_2}{\hbar k_z''} \right] R^{FB}(\mathbf{k}''; \mathbf{k}') \right\} f_{\text{in}}^B(\mathbf{k}'), \end{aligned} \quad (86b)$$

$$\begin{aligned} \tau_{B \leftarrow B}^{\text{out}}(z_1) &= \iiint_{\text{open}} d^3 k \iiint_{\text{open}} d^3 k' \left\{ f_{\text{in}}^B(\mathbf{k})^* \iiint_{\text{open}} d^3 k'' T^{BB}(\mathbf{k}''; \mathbf{k})^* \right. \\ &\times \left. \left[-\frac{1}{i} \frac{\partial}{\partial k_t''} + \frac{mz_1}{\hbar k_z''} \right] T^{BB}(\mathbf{k}''; \mathbf{k}') \right\}. \end{aligned} \quad (86c)$$

We now undertake to use the derived results to obtain estimates for the average delay time for the four processes of transmission and reflection. Due to the absence of space- and time-reversal symmetry of the potential energy, there will be no special relationships between the two transmission times or between the two reflection times. Let the transmission delay times be called $\tau_{F \leftarrow F}^{\text{trans}}(z_2 \leftarrow z_1)$ and $\tau_{B \leftarrow B}^{\text{trans}}(z_1 \leftarrow z_2)$, while the reflection delay times are called $\tau_{F \leftarrow F}^{\text{refl}}(z_1 \leftarrow z_1)$ and $\tau_{B \leftarrow B}^{\text{refl}}(z_2 \leftarrow z_2)$. We proceed from the following principle for computing delay times (currents are taken with their algebraic signs intact):

$$\begin{aligned} \text{delay time} = & \frac{(\text{output current of time at exit point})}{(\text{output particle current at exit point})} \\ & - \frac{(\text{input current of time at entry point})}{(\text{input particle current at entry point})}, \end{aligned} \quad (87)$$

where the exit point is the same, or the opposite, as the entry point (i.e., z_1 or z_2) on reflection, or on transmission, respectively. We therefore have that

$$\tau_{F \leftarrow F}^{\text{trans}}(z_2 \leftarrow z_1) = \frac{\tau_{F \leftarrow F}^{\text{out}}(z_2)}{\mathcal{T}_{F \leftarrow F}^{\text{out}}(z_2)} - \tau_F^{\text{in}}(z_1), \quad (88\text{a})$$

$$\tau_{B \leftarrow F}^{\text{refl}}(z_1 \leftarrow z_1) = \frac{\tau_{B \leftarrow F}^{\text{out}}(z_1)}{\mathcal{R}_{B \leftarrow F}^{\text{out}}(z_1)} - \tau_F^{\text{in}}(z_1), \quad (88\text{b})$$

$$\tau_{B \leftarrow B}^{\text{trans}}(z_1 \leftarrow z_2) = \frac{\tau_{B \leftarrow B}^{\text{out}}(z_1)}{\mathcal{T}_{B \leftarrow B}^{\text{out}}(z_1)} + \tau_B^{\text{in}}(z_2), \quad (88\text{c})$$

$$\tau_{F \leftarrow B}^{\text{refl}}(z_2 \leftarrow z_2) = \frac{\tau_{F \leftarrow B}^{\text{out}}(z_2)}{\mathcal{R}_{F \leftarrow B}^{\text{out}}(z_2)} + \tau_B^{\text{in}}(z_2). \quad (88\text{d})$$

General formulas for estimates of these delay times in first-order perturbation theory for weak potentials are derived in the appendix.

4 Applications to s-waves and a step potential

In this section we obtain expressions for the dwell times first, for s-wave scattering so that z can be regarded as a radial coordinate, and second, delay times in scattering from a t, x, y -independent step potential barrier in the z -direction.

Let us now consider the simple problem of scattering from an infinite potential barrier at $z_1 = 0$ with $z_2 > 0$ in an open and separately in a closed-channel case. The dwell time and the delay time for reflection are equal. The input is now controlled by $f_{\text{in}}^B(\mathbf{k})$; we infer from Eqs. (45b), (33), (36), and (38) that, in order that the first component of $\Psi(t, x, y, 0)$ be zero for all t, x, y , we must have

$$f_{\text{out}}^F(\mathbf{k}) = -f_{\text{in}}^B(\mathbf{k}), \quad \text{for open channels,} \quad (89\text{a})$$

$$f_{\text{out}}^F(\mathbf{k}) = -if_{\text{in}}^B(\mathbf{k}), \quad \text{for closed channels.} \quad (89\text{b})$$

The expectation value of $\langle \tilde{t}I_2 \rangle$ is then zero at $z_1 = 0$. we infer for open-channel input that the dwell time is

$$\begin{aligned}\langle \tilde{t}I_2 \rangle_{\Psi(z_2)} &= \iiint_{\text{open}} d^3k |f_{\text{in}}^B(\mathbf{k})|^2 \left[\frac{2mz_2}{\hbar k_z} - \frac{m}{\hbar k_z^2} \sin(2k_z z_2) \right] \\ &\approx \iiint_{\text{open}} d^3k |f_{\text{in}}^B(\mathbf{k})|^2 \frac{4mk_z z_2^3}{3\hbar}, \quad \text{as } z_2 \rightarrow 0,\end{aligned}\quad (90)$$

while for closed-channel input that the dwell time is

$$\begin{aligned}\langle \tilde{t}I_2 \rangle_{\Psi(z_2)} &= \iiint_{\text{closed}} d^3k |f_{\text{in}}^B(\mathbf{k})|^2 \left[-\frac{2mz_2}{\hbar \kappa_z} + \frac{m}{\hbar \kappa_z^2} \sinh(2\kappa_z z_2) \right] \\ &\approx \iiint_{\text{closed}} d^3k |f_{\text{in}}^B(\mathbf{k})|^2 \frac{4m\kappa_z z_2^3}{3\hbar}, \quad \text{as } z_2 \rightarrow 0.\end{aligned}\quad (91)$$

In the open-channel case we have an oscillatory contribution to the dwell time that is of diminishing relative importance as z_2 becomes large. In this computation, the dwell time contains interference terms between the input and output waves. If these interference terms are dropped, only the first term, which is proportional to z_2 , survives in the square brackets first rhs of Eq. (90), and the time delay on reflection is the distance traveled ($2z_2$) times the average of the reciprocal of the speed of travel ($m/\hbar k_z$).

Next, we generalize to case that again there is a large potential barrier to the left of $z_1 = 0$ so that the transmission coefficients $T^{BB}(\mathbf{k}; \mathbf{k}')$ are zero: The expectation value $\langle tI \rangle_{\Psi(0)}$ is again zero. However, we assume an additional potential $V(t, x, y, z)$, the support of which is contained in the interval $[0, z_2]$, and an open-channel input amplitude $f_{\text{in}}^B(\mathbf{k})$ with no input from the left, that is, $f_{\text{in}}^F(\mathbf{k}) \equiv 0$. The reflection coefficients $R^{FB}(\mathbf{k}; \mathbf{k}')$ now comprise minus the usual S -matrix elements for scattering from the potential+barrier. We infer from Eqs. (70) and (74) that

$$\begin{aligned}\langle \tilde{t}I_2 \rangle_{\Psi(z)} &= \iiint_{\text{open}} d^3k \left[\frac{mz_2}{\hbar k_z} |f_{\text{in}}^B(\mathbf{k})|^2 - f_{\text{in}}^B(\mathbf{k})^* \frac{1}{i} \frac{\partial f_{\text{in}}^B}{\partial k_t}(\mathbf{k}) \right] \\ &+ \iiint_{\text{open}} d^3k \iiint_{\text{open}} d^3k' f_{\text{in}}^B(\mathbf{k})^* \left\{ -\frac{im}{2\hbar k_z^2} \exp(2ik_z z_2) R^{FB}(\mathbf{k}; \mathbf{k}') \right. \\ &+ R^{FB}(\mathbf{k}'; \mathbf{k})^* \frac{im}{2\hbar k_z'^2} \exp(-2ik_z' z_2) \\ &+ \iiint_{\text{open}} d^3k'' R^{FB}(\mathbf{k}''; \mathbf{k})^* \left[\frac{mz_2}{\hbar k_z''} + \frac{1}{i} \frac{\partial}{\partial k_t''} \right] R^{FB}(\mathbf{k}''; \mathbf{k}') \\ &- \iiint_{\text{closed}} d^3k'' R^{FB}(\mathbf{k}''; \mathbf{k})^* \\ &\times \left. \left. \times \frac{m}{2\hbar k_z''^2} \exp(-2\kappa_z'' z_2) R^{FB}(\mathbf{k}''; \mathbf{k}') \right\} f_{\text{in}}^B(\mathbf{k}'). \right.\end{aligned}\quad (92)$$

In the above, the term involving $R^{FB}(\mathbf{k}''; \mathbf{k})^*(-i)\partial R^{FB}/\partial k_t''(\mathbf{k}'')$ reduces to the familiar $S^\dagger(-i\hbar)\partial S/\partial E$ that has been derived as the extra dwell time for a scattering process in the presence of a time-independent potential—see Eq. (44) in Smith [30]. Note that in his Eq. (37) and otherwise, Smith defines initial-to-final index labels of the S -matrix and collision-lifetime matrix Q from left to right, the opposite of what is done here for input-to-output labels. The terms proportional to z_2 are a generalized version of the “background” average of $2z_2/(z\text{-speed})$ as the dwell term for a non-interacting case; note that one of the two contributions to the background time delay nevertheless involves the S -matrix.

The remaining terms on the rhs of Eq. (92) do not enter the traditional formulas: In particular, the terms with D_2 in Eq. (76) involve interference between the input and output waves at the points $z = z_1$ or $z = z_2$ where a measurement is made. Note the presence in $D_2(\dagger)$ of factors of the form $\exp(\pm 2ik_z' z_1)$ or $\exp(\pm 2ik_z' z_2)$; for a macroscopically large z_1 and z_2 , these factors will be rapidly oscillating in k_z' , and cause the effective cancellation of such contributions for all but extremely monochromatic and planar incoming and outgoing wave packets. Note also that the closed-channel contributions tend to zero exponentially in Eq. (80) as z_2 increases and z_1 decreases away from the scattering region.

We now assume that there is a finite, t, x, y -independent potential barrier of the generic type used by Bohm ([31], Fig. 17) but which can be attractive or repulsive. Choose a real number K , of physical dimension time^{-1} , and a positive length a such that

$$V(t, x, y, z) = \begin{cases} \hbar K, & \forall t, x, y, \text{ for } -a < z < a, \\ 0, & \text{otherwise.} \end{cases} \quad (93)$$

Given open-channel input only, we first define the vector $\tilde{\mathbf{k}}$ as

$$(\tilde{\mathbf{k}}) = (\tilde{k}_t, \tilde{k}_x, \tilde{k}_y) = (k_t - K, k_x, k_y), \quad (94)$$

and also

$$\begin{aligned} \tilde{k}_z &= \left[\frac{2m}{\hbar^2} \tilde{k}_t - \tilde{k}_x^2 - \tilde{k}_y^2 \right]^{1/2}, \\ \tilde{\kappa}_z &= \left[\tilde{k}_x^2 + \tilde{k}_y^2 - \frac{2m}{\hbar^2} \tilde{k}_t \right]^{1/2}, \end{aligned} \quad (95)$$

when the particle can or cannot, respectively, pass over the top of the barrier classically. When $K > 0$, we shall obtain the intermediate case $\tilde{k}_z = 0$ or $\tilde{\kappa}_z = 0$ by limiting processes; the result of both limits will be the same solution to the Schrödinger equation, so that there is a continuity between the above-the-barrier and below-the-barrier S -matrices.

We shall omit the details of the derivation, and state the results of a computation of the S -matrix:

$$S(\mathbf{k}; \mathbf{k}') = s(\mathbf{k}) \otimes I^{\text{open}}(\mathbf{k} - \mathbf{k}'), \quad (96)$$

where the 2×2 matrix $s(\mathbf{k})$ is written

$$s(\mathbf{k}) = \begin{bmatrix} t^{FF}(\mathbf{k}) & r^{FB}(\mathbf{k}) \\ r^{BF}(\mathbf{k}) & t^{BB}(\mathbf{k}) \end{bmatrix}. \quad (97)$$

When $K \leq 0$, or when $K > 0$ with \mathbf{k} above the barrier, we obtain the following components for the s -matrix, denoted with a subscript abv:

$$t_{\text{abv}}^{FF} = t_{\text{abv}}^{BB} = \exp(-2ik_z a) \left[\cos(2\tilde{k}_z a) - \frac{i}{2} \left(\frac{\tilde{k}_z}{k_z} + \frac{k_z}{\tilde{k}_z} \right) \sin(2\tilde{k}_z a) \right]^{-1}, \quad (98a)$$

$$r_{\text{abv}}^{FB} = r_{\text{abv}}^{BF} = \frac{i}{2} \left(\frac{\tilde{k}_z}{k_z} - \frac{k_z}{\tilde{k}_z} \right) \sin(2\tilde{k}_z a) t_{\text{abv}}^{FF}. \quad (98b)$$

For $K > 0$ and \mathbf{k} below the barrier, we find the s -matrix components, denoted by a subscript bel, to be

$$t_{\text{bel}}^{FF} = t_{\text{bel}}^{BB} = \exp(-2ik_z a) \left[\cosh(2\tilde{\kappa}_z a) + \frac{i}{2} \left(\frac{\tilde{\kappa}_z}{k_z} - \frac{k_z}{\tilde{\kappa}_z} \right) \sinh(2\tilde{\kappa}_z a) \right]^{-1}, \quad (99a)$$

$$r_{\text{bel}}^{FB} = r_{\text{bel}}^{BF} = -\frac{i}{2} \left(\frac{\tilde{\kappa}_z}{k_z} + \frac{k_z}{\tilde{\kappa}_z} \right) \sinh(2\tilde{\kappa}_z a) t_{\text{bel}}^{FF}. \quad (99b)$$

Note that both s -matrices are unitary for each \mathbf{k} , and that there is continuity of the results between $\tilde{k}_z \rightarrow 0$ and $\tilde{\kappa}_z \rightarrow 0$.

We shall compute delay times for transmission across, and reflection from, the step potential according to Eq. (88). In order to evaluate the terms involving derivatives of the s -matrix and input amplitudes in a convenient form, we can, after dropping perfect divergences, obtain

$$\begin{aligned} & \iiint_{\text{open}} d^3 k f(\mathbf{k})^* t(\mathbf{k})^* \frac{1}{i} \frac{\partial}{\partial k_t} [f(\mathbf{k}) t(\mathbf{k})] \\ &= \iiint_{\text{open}} d^3 k |f(\mathbf{k}) t(\mathbf{k})|^2 \Im \left[\frac{\partial}{\partial k_t} \ln(f(\mathbf{k}) t(\mathbf{k})) \right], \end{aligned} \quad (100)$$

where \Im means “imaginary part of”.

A computation shows that the imaginary part of the k_t -derivative of the logarithm of $t^{FF}(\mathbf{k})$, $r^{BF}(\mathbf{k})$, $r^{FB}(\mathbf{k})$, and $t^{BB}(\mathbf{k})$ are all the same, which result we call $\Delta(\mathbf{k})$. We omit the calculational details, and give the result:

$$\begin{aligned} \Im \frac{\partial}{\partial k_t} \ln[t^{FF}(\mathbf{k})] &= \Delta(\mathbf{k}) \\ &= \begin{cases} -\frac{2ma}{\hbar k_z} + |t^{FF}(\mathbf{k})|^2 \left[\frac{ma}{\hbar k_z} \left(\frac{\tilde{k}_z}{k_z} + \frac{k_z}{\tilde{k}_z} \right) \right. \\ \left. - \frac{m}{4\hbar k_z \tilde{k}_z} \left(\frac{\tilde{k}_z}{k_z} - \frac{k_z}{\tilde{k}_z} \right)^2 \sin(4\tilde{k}_z a) \right], & \mathbf{k} \text{ above barrier}, \\ -\frac{2ma}{\hbar k_z} + |t^{FF}(\mathbf{k})|^2 \left[\frac{ma}{\hbar \tilde{\kappa}_z} \left(\frac{\tilde{\kappa}_z}{k_z} - \frac{k_z}{\tilde{\kappa}_z} \right) \right. \\ \left. - \frac{m}{4\hbar k_z \tilde{\kappa}_z} \left(\frac{\tilde{\kappa}_z}{k_z} + \frac{k_z}{\tilde{\kappa}_z} \right)^2 \sinh(4\tilde{\kappa}_z a) \right], & \mathbf{k} \text{ below barrier}. \end{cases} \end{aligned} \quad (101)$$

Referring to Eq. (88), we can now compute the delay times upon transmission and reflection for left and right input, assuming the overall input is normalized as in (47). In the present case the reflected and transmitted currents of particle presence of Eqs. (81) and (84) reduce to

$$\mathcal{R}_{B \leftarrow F}^{\text{out}}(z_1) = - \iiint_{\text{open}} d^3 k |f_{\text{in}}^F(\mathbf{k}) r^{BF}(\mathbf{k})|^2, \quad (102\text{a})$$

$$\mathcal{T}_{F \leftarrow F}^{\text{out}}(z_2) = \iiint_{\text{open}} d^3 k |f_{\text{in}}^F(\mathbf{k}) t^{FF}(\mathbf{k})|^2, \quad (102\text{b})$$

$$\mathcal{R}_{F \leftarrow B}^{\text{out}}(z_2) = \iiint_{\text{open}} d^3 k |f_{\text{in}}^B(\mathbf{k}) r^{FB}(\mathbf{k})|^2, \quad (102\text{c})$$

$$\mathcal{T}_{B \leftarrow B}^{\text{out}}(z_1) = - \iiint_{\text{open}} d^3 k |f_{\text{in}}^B(\mathbf{k}) t^{BB}(\mathbf{k})|^2; \quad (102\text{d})$$

note that backward-flowing currents, whether on input or output, are negative. Also, we find that the input currents of time are, from Eqs. (83a) and (86a),

$$\tau_F^{\text{in}}(z_1) = \iiint_{\text{open}} d^3 k |f_{\text{in}}^F(\mathbf{k})|^2 \left[\Im \left(\frac{\partial}{\partial k_t} \ln [f_{\text{in}}^F(\mathbf{k})] \right) + \frac{m z_1}{\hbar k_z} \right], \quad (103\text{a})$$

$$\tau_B^{\text{in}}(z_2) = \iiint_{\text{open}} d^3 k |f_{\text{in}}^F(\mathbf{k})|^2 \left[-\Im \left(\frac{\partial}{\partial k_t} \ln [f_{\text{in}}^B(\mathbf{k})] \right) + \frac{m z_2}{\hbar k_z} \right]. \quad (103\text{b})$$

The average delay times are

$$\begin{aligned} \tau_{F \leftarrow F}^{\text{trans}}(z_2 \leftarrow z_1) &= [\mathcal{T}_{F \leftarrow F}^{\text{out}}(z_1)]^{-1} \iiint_{\text{open}} d^3 k |f_{\text{in}}^F(\mathbf{k}) t^{FF}(\mathbf{k})|^2 \left[\Delta(\mathbf{k}) \right. \\ &\quad \left. + \Im \left(\frac{\partial}{\partial k_t} \ln [f_{\text{in}}^F(\mathbf{k})] \right) + \frac{m z_2}{\hbar k_z} \right] - \tau_F^{\text{in}}(z_1), \end{aligned} \quad (104\text{a})$$

$$\begin{aligned} \tau_{B \leftarrow F}^{\text{refl}}(z_1 \leftarrow z_1) &= [\mathcal{R}_{B \leftarrow F}^{\text{out}}(z_1)]^{-1} \iiint_{\text{open}} d^3 k |f_{\text{in}}^F(\mathbf{k}) t^{FF}(\mathbf{k})|^2 \left[-\Delta(\mathbf{k}) \right. \\ &\quad \left. - \Im \left(\frac{\partial}{\partial k_t} \ln [f_{\text{in}}^F(\mathbf{k})] \right) + \frac{m z_1}{\hbar k_z} \right] - \tau_F^{\text{in}}(z_1), \end{aligned} \quad (104\text{b})$$

$$\begin{aligned} \tau_{B \leftarrow B}^{\text{trans}}(z_1 \leftarrow z_2) &= [\mathcal{T}_{B \leftarrow B}^{\text{out}}(z_1)]^{-1} \iiint_{\text{open}} d^3 k |f_{\text{in}}^B(\mathbf{k}) t^{BB}(\mathbf{k})|^2 \left[-\Delta(\mathbf{k}) \right. \\ &\quad \left. - \Im \left(\frac{\partial}{\partial k_t} \ln [f_{\text{in}}^B(\mathbf{k})] \right) + \frac{m z_1}{\hbar k_z} \right] + \tau_B^{\text{in}}(z_2), \end{aligned} \quad (104\text{c})$$

$$\begin{aligned} \tau_{F \leftarrow B}^{\text{refl}}(z_2 \leftarrow z_2) &= [\mathcal{R}_{F \leftarrow B}^{\text{out}}(z_2)]^{-1} \iiint_{\text{open}} d^3 k |f_{\text{in}}^B(\mathbf{k}) r^{FB}(\mathbf{k})|^2 \left[\Delta(\mathbf{k}) \right. \\ &\quad \left. + \Im \left(\frac{\partial}{\partial k_t} \ln [f_{\text{in}}^B(\mathbf{k})] \right) + \frac{m z_2}{\hbar k_z} \right] + \tau_B^{\text{in}}(z_2). \end{aligned} \quad (104\text{d})$$

Suppose that the input amplitudes $f_{\text{in}}^{\zeta}(\mathbf{k})$ are real and are concentrated about an open-channel value \mathbf{k}^0 . Presuming also that the reflection and transmission

coefficients are slowly varying, we can assume them to be constant in the neighborhood of \mathbf{k}^0 . The delay times of Eq. (104) then take the approximate forms

$$\tau_{F \leftarrow F}^{\text{trans}}(z_2 \leftarrow z_1) = \Delta(\mathbf{k}^0) + \frac{m(z_2 - z_1)}{\hbar k_z^0}, \quad (105\text{a})$$

$$\tau_{B \leftarrow F}^{\text{refl}}(z_1 \leftarrow z_1) = \Delta(\mathbf{k}^0) - \frac{2mz_1}{\hbar k_z^0}, \quad (105\text{b})$$

$$\tau_{B \leftarrow B}^{\text{trans}}(z_1 \leftarrow z_2) = \Delta(\mathbf{k}^0) + \frac{m(z_2 - z_1)}{\hbar k_z^0}, \quad (105\text{c})$$

$$\tau_{F \leftarrow B}^{\text{refl}}(z_2 \leftarrow z_2) = \Delta(\mathbf{k}^0) + \frac{2mz_2}{\hbar k_z^0}. \quad (105\text{d})$$

The function $\Delta(\mathbf{k}^0)$ therefore corresponds to the extra time delay in transmission as defined by Bohm ([31], Ch. 11.19, Eqs. (82) and (83)). We note also that Eqs. (105a) and (105b) resemble the formulas of Ref. [10], Eqs. (10) and (11)—they position the barrier between $x = 0$ and $x = a$ —except for the term in their Eq. (10) that adds ka to $\arg(A_T)$ (i.e., adds $2k_z^0 a$ to $\arg(t^{FF})$ in the present notation): this part of their formula cannot be valid, as it yields an incorrect answer when $t^{FF} \equiv 1$, as is the case when the barrier height is zero.

Bohm's result was formulated for an attractive well, but also holds for a repulsive well so long as the incoming wave vector is above the barrier; that result diverges, as does the classical result, for the transmission time for a particle grazing the top of a repulsive barrier. The function $\Delta(\mathbf{k}^0)$ differs from Bohm's time delay, in that it remains finite as \mathbf{k}^0 approaches the top of the barrier, and it is defined for values of \mathbf{k}^0 below the barrier. In fact we find, as \mathbf{k}^0 approaches the barrier from values both above and below, that

$$\Delta(\mathbf{k}_0) \rightarrow \frac{ma}{\hbar k_z^0} [1 - 2(k_z^0 a)^2] [1 + (k_z^0 a)^2]^{-1}. \quad (106)$$

This result also disagrees with that obtained in Ref. [10], Eqs. (12b) and (13b), by the stationary phase method: if we put $z_2 = a$ and $z_1 = -a$ in Eq. (105a), we find

$$\tau_{F \leftarrow F}^{\text{trans}}(+a \leftarrow -a) = \frac{3ma}{\hbar k_z^0} [1 + (k_z^0 a)^2]^{-1}, \quad (107)$$

which has a different dependence on k_z^0 and a from the result in [10]. The result [10], Eq. (12b), taken for thin barriers, resembles the last rhs of (90), above, where there is reflection from an infinite wall at $z_1 = 0$, and interference between backward and forward propagating signals in the computation of the time delay. As stated in [10], in a paragraph between Eqs. (12a) and (13a), those authors have not avoided the interference effects between incident and reflected waves in computing their phase times.

It is also of interest to find the time delay for transmission as the barrier height $\hbar K$ becomes large, while \mathbf{k}^0 remains fixed. We find that

$$\Delta(\mathbf{k}^0) \rightarrow \frac{2m}{\hbar k_z \tilde{\kappa}_z}, \quad \text{as } \tilde{\kappa}_z \rightarrow \infty. \quad (108)$$

This result coincides with the asymptotic group delay (Ref. [12], p. 352, and [32], Eq. (13')). Remarkably, the transmission delay time tends to zero as the barrier gets higher—at least, until relativistic effects intervene. However, the transmission probability behaves as $4(k_z/\bar{\kappa}_z)^2 \exp(-4\bar{\kappa}_z a)$ in the same region, so that proportionately very few particles cross the barrier.

5 Discussion

We begin this section by reëmphasizing that it is the Schrödinger equation that is taken as fundamental in the present argument, and that a theory of measurement, a probability interpretation, and an uncertainty principle, are all presumed to be derivative ideas that may require alterations from their conventional forms in order to bring them into concord with the body of formalism presented here.

In particular, we have relinquished the notion that the norm of a Schrödinger wave function, in problems involving input on the spatial walls of a region, represents a probability in a straightforward sense: this norm is a net average current of particles across a surface. More precisely, if a large number of trials is made with the same input, the norm Eq. (15) represents a net particle transit count across a $z=\text{constant}$ plane divided by the number of trials, and Eq. (13) represents the normalized density of such counts (per unit spatial area per unit time); in making a transit count, particles are counted positively or negatively as they pass across the given z -plane in a positive or negative direction. The Schrödinger equation can create spatially and temporally localized eddies of probability current: even though a wave is made up entirely of a packet of F -type open-channel states, this current density can be negative in a neighborhood—see the examples cited below—and therefore will be greater than one in a complementary set of the given $z=\text{constant}$ plane. Hence, even for a packet of only free-particle F -type states this normalized particle count can fall outside the interval $[0, 1]$ on proper subsets of a $z=\text{constant}$ plane, and is not a probability, although a transition process, as in the conventional interpretation of quantum mechanics, has irreducible randomness and is unpredictable in detail in contrast to a classical process. A further complication results from the circumstance that this normalized particle count is not, when closed channels are present, even globally (i.e., across an entire $z=\text{constant}$ plane) an algebraic sum of two separate currents due to forward- and backward-moving particles, as there can be nonzero global interference between the F - and B -type closed-channel contributions to the total current.

Since the sum of the projection operators for F - and B -type states—see Eq. (111)—is the unit operator on a $z=\text{constant}$ plane, it is possible, with the given physical system, to make a measurement of local ((t, x, y)) net transit flux of particles across a proper subset of the plane. A local measurement of either the positive or the negative direction in z of a particle's transit involves non-commuting projection operators, one in position space and one in wavenumber space. That is, we would then ask two incompatible yes/no questions: (1) Did

the particle cross the plane in a given proper (t, x, y) subregion? (2) Did the particle cross positively/negatively in the z -direction? The outcome depends on the details of an often-repeated measurement on the system with the same input in each trial. To be sure, taking a sufficiently large subset of the $z=\text{constant}$ plane for asking question (1) will, to a good approximation, be close to taking all of it, so that question (2) can be answered with negligible inconsistency. Also, the question “What is the difference between the numbers of particles crossing positively and particles crossing negatively across a small subregion of the z -plane?” involves no inconsistency, and yields a result predictable from the wave function alone; it is the separate local densities of positive and of negative crossings, not their difference, that depend on the measurement scheme.

When closed-channel amplitudes are negligible, a probability interpretation in the mapping of input into output on two $z=\text{constant}$ planes is feasible, due to the unitarity of the open-channel S_o -matrix of Eq. (62a).

A substantial effort has been dedicated to the establishment of a time-energy uncertainty principle—see the discussion and references in [33]. An uncertainty principle appears to be associated with a positive definite metric, a requirement that we have dropped. It is not obviously impossible to formulate some kind of a time-energy uncertainty principle within the present formalism in special circumstances, but we shall not investigate this subject here.

Kijowski [16], [34] undertook to establish a time-energy uncertainty principle by analyzing the evolution of a Schrödinger wave function in a space-like direction, and in this respect there is overlap between Kijowski’s work and the present undertaking. Kijowski’s first “unsuccessful attempt” ([16], §3) begins in a similar manner as that proposed above, but his inner product law does not involve an integral over time; since, as noted following Eq. (37), the wave functions of Eq. (36) do not satisfy the Cauchy inequality, the interference terms in a local inner product can make the current density negative for the superposition of two forward-traveling states, as shown in an example in [16], §3. Mielnik ([18], §5, Lemma) noted that a Schrödinger wave packet that at $t = 0$ has its source entirely to the left of $z = 0$, say, could eventually give rise to probability currents normal to the $z = 0$ plane that need not be everywhere positive. Similarly, the integrand for the particle current for the norm of a superposition of F -type open-channel states in Eq. (15) need not be everywhere nonnegative. These local negative currents all result from interference terms that yield zero net contribution in the present formalism due to the integral over t , x and y in the inner product.

Kijowski’s formalism is substantially different from the present one—the norm of an F -type state is given in [16], Eq. (9)—but in which the average time of crossing a spacelike wall for F -type states nevertheless reduces to the same form ([16], §10) in terms of the probability current as Eq. (24). There are discussions of Kijowski’s work in [35], §1.5.1, and [36], §10.2.

Mielnik [18] critiques both Kijowski’s [16] and Piron’s [17] attempts to establish formalisms for spacewise propagation of a wave function, concludes that they do not offer a solution to the problem of defining time as an observable, and makes no additional proposals along these lines. Although the initial ideas

of the two latter papers resemble that of the present paper, the respective implementations differ considerably, so we shall not attempt further review of them here.

Another question concerns the generalization of the effect of a measurement on a wave function that propagates in both directions across the surface on which the measurement is performed. Suppose in fact that, in a problem of type II, two adjacent boxes occupy the space-like intervals $[z_1, z_2]$ and $[z_2, z_3]$, and that a measurement is made (over t, x, y) at $z = z_2$, which measurement partly “collapses” the wave function there. The input at z_2 to both boxes can change directly or indirectly as a result of the acquired information, leading in turn to a change in the overall output at z_1 and z_3 , and, due to reflections, a change in the wave function at z_2 at which the measurement is made. There is therefore a problem of consistency, in that the measurement at z_2 indirectly changes the wave function at z_2 and therefore changes the frequency of results of the measurement at z_2 , and so on. This problem is analogous to the “grandfather paradox” (see [37], Ch. 4) of the influence of a physical system with itself between two different $t=\text{constant}$ surfaces when two-way interaction occurs. No attempt at analysis of this problem will be made here.

To recapitulate, the conventional probability interpretation derived from the Schrödinger wave function does not seem to apply when problems of type II are confronted. The claim is that the wave function in type II problems does permit the computation of certain expectation values, that is, average results of many repeated experiments with the same input signal. An interpretation involving randomness of a more general nature than that which can be characterized by probabilities seems called for. We infer that the conventional interpretation should be subordinated to an interpretation involving stochastic currents of particle presence, and, more comprehensively, stochastic currents of other physical quantities as temporal position, spatial position, energy, momentum, and so on. This “particle current” interpretation of the formalism can describe systems of both types I and II; the usual probability interpretation then applies in problems of type I and other special cases. Although what appears to be a mathematically consistent formalism has been constructed herein, and a preliminary physical interpretation advanced, many questions along these lines need to be addressed, and consistency with experimental tests established, before the proposal can with confidence be regarded as a physical theory.

The above limitations notwithstanding, the formalism proposed herein has obtained results that agree to an extent with some special results previously derived, and has secured results that would be difficult to obtain by other published methods of analysis: for example, a generic expression Eqs. (75)–(80) for the average dwell time for a particle reflecting from or passing through a time-dependent barrier.

6 Appendix: Perturbation theory

We want to obtain the dwell times for a signal impinging on a weak potential, which diminishes rapidly in absolute value as $|t|$ or $|x|$ or $|y|$ tend to infinity, to first order in perturbation theory. Remarks at the end deal with delay times in the same circumstance.

We define H_0 and its adjoint operator $(H_0)_{\text{adj}}$ following Eq. (11):

$$H_0 = \begin{bmatrix} 0 & \frac{2mi}{\hbar^2} \\ \hbar \frac{\partial}{\partial t} - \frac{i\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) & 0 \end{bmatrix}, \quad (109a)$$

$$(H_0)_{\text{adj}} = \begin{bmatrix} 0 & \hbar \frac{\partial}{\partial t} + \frac{i\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \\ -\frac{2mi}{\hbar^2} & 0 \end{bmatrix}; \quad (109b)$$

$(H_0)_{\text{adj}}$ differs from $(H_0)^\dagger$ by changing the signs of the partial derivatives and making them act to the left, as indicated by the arrows. We also define projection operators for free-particle solutions, making use of Eq. (44):

$$\begin{aligned} P^F(z; t', x', y'; t, x, y) &= \hbar^{-1} \iiint_{\text{open}} d^3 k \Xi^F(\mathbf{k}; t', x', y', z) \Xi^F(\mathbf{k}; t, x, y, z)^\dagger M \\ &\quad + \hbar^{-1} \iiint_{\text{closed}} d^3 k \Xi^F(\mathbf{k}; t', x', y', z) \Xi^B(\mathbf{k}; t, x, y, z)^\dagger M, \end{aligned} \quad (110a)$$

$$\begin{aligned} P^B(z; t', x', y'; t, x, y) &= -\hbar^{-1} \iiint_{\text{open}} d^3 k \Xi^B(\mathbf{k}; t', x', y', z) \Xi^B(\mathbf{k}; t, x, y, z)^\dagger M \\ &\quad + \hbar^{-1} \iiint_{\text{closed}} d^3 k \Xi^B(\mathbf{k}; t', x', y', z) \Xi^F(\mathbf{k}; t, x, y, z)^\dagger M. \end{aligned} \quad (110b)$$

It can be shown that P^F and P^B are independent of z , and that

$$P^F(z; t', x', y'; t, x, y) + P^B(z; t', x', y'; t, x, y) = I_2 \otimes \delta(t' - t) \delta(x' - x) \delta(y' - y). \quad (111)$$

Let us obtain the causal Green's function $G_0^{(+)}$ for the adjoint to Eq. (3) with $V(t, x, y, z) \equiv 0$, in complete space-time:

$$\begin{aligned} -\frac{\hbar}{i} \frac{\partial}{\partial z} G_0^{(+)}(t', x', y', z'; t, x, y, z) - G_0^{(+)}(t', x', y', z'; t, x, y, z) M(H_0)_{\text{adj}} M \\ = I_2 \otimes \delta(t' - t) \delta(x' - x) \delta(y' - y) \delta(z' - z). \end{aligned} \quad (112)$$

This Green's function proves to be

$$\begin{aligned}
G_0^{(+)}(t', x', y', z'; t, x, y, z) &= \frac{i}{\hbar} \iiint_{\text{open}} d^3 k \left[\theta(z' - z) \Xi^F(\mathbf{k}; t', x', y', z') \Xi^F(\mathbf{k}; t, x, y, z)^\dagger M \right. \\
&\quad + \theta(z - z') \Xi^B(\mathbf{k}; t', x', y', z') \Xi^B(\mathbf{k}; t, x, y, z)^\dagger M \Big] \\
&\quad + \frac{i}{\hbar} \iiint_{\text{closed}} d^3 k \left[\theta(z' - z) \Xi^F(\mathbf{k}; t', x', y', z') \Xi^B(\mathbf{k}; t, x, y, z)^\dagger M \right. \\
&\quad \left. - \theta(z - z') \Xi^B(\mathbf{k}; t', x', y', z') \Xi^F(\mathbf{k}; t, x, y, z)^\dagger M \right].
\end{aligned} \tag{113}$$

This Green's function can be derived from the usual Feynman-type free-particle kernel ([38], Eq. (5.12)), and is therefore causal in time.

Let $\Psi_0(t, x, y, z)$ be a solution to the free-particle Schrödinger equation in a region covering \mathcal{B}_2 and its boundary, and $\Psi(t, x, y, z)$ be a solution to the Schrödinger equation with a generic interaction Hamiltonian H_1 in the same region:

$$\frac{1}{i} \frac{\partial \Psi_0}{\partial z}(t, x, y, z) - H_0 \Psi_0(t, x, y, z) = 0, \tag{114a}$$

$$\frac{1}{i} \frac{\partial \Psi}{\partial z}(t, x, y, z) - H_0 \Psi(t, x, y, z) - H_1 \Psi(t, x, y, z) = 0. \tag{114b}$$

The H_1 derived from Eq. (3) is

$$H_1 = \begin{bmatrix} 0 & 0 \\ iV(t, x, y, z) & 0 \end{bmatrix}, \tag{115}$$

but more general cases occur if magnetic fields are present and the particle is charged. Standard manipulations on Eqs. (112) and (114) now yield, for $(t', x', y', z') \in \mathcal{B}_2$,

$$\begin{aligned}
\Psi(t', x', y', z') &= \Psi_0(t', x', y', z') + \iiint_{\mathcal{B}_2} dt dx dy dz \\
&\quad \times G_0^{(+)}(t', x', y', z'; t, x, y, z) [M(H_0)_{\text{adj}} M - H_0] \\
&\quad \times [\Psi(t, x, y, z) - \Psi_0(t, x, y, z)] + i \left\{ \iiint_{\mathbb{R}^3} dt dx dy \right. \\
&\quad \times G_0^{(+)}(t', x', y', z'; t, x, y, z) \\
&\quad \times [\Psi(t, x, y, z) - \Psi_0(t, x, y, z)] \Big\}_{z=z_1}^{z=z_2} + \iiint_{\mathcal{B}_2} dt dx dy dz \\
&\quad \times G_0^{(+)}(t', x', y', z'; t, x, y, z) H_1 \Psi(t, x, y, z).
\end{aligned} \tag{116}$$

The first term on the rhs disappears after an integration by parts on t, x, y , since $M(H_0)^\dagger M - H_0 = 0$. The second term on the rhs, involving triple integrals at

$z = z_1$ and $z = z_2$, vanishes since $\Psi(t, x, y, z) - \Psi_0(t, x, y, z)$ self-consistently has only outgoing waves at $z = z_1$ and at $z = z_2$, while scrutiny of Eq. (113) indicates that, since $z_1 < z' < z_2$, these contributions are annihilated by the Green's function. Hence, we obtain an integral equation for Ψ that readily yields a perturbation expansion in powers of H_1 :

$$\begin{aligned}\Psi(t', x', y', z') &= \Psi_0(t', x', y', z') \\ &+ \iiint_{B_2} dt dx dy dz G_0^{(+)}(t', x', y', z'; t, x, y, z) H_1 \Psi(t, x, y, z).\end{aligned}\quad (117)$$

We substitute

$$\Psi(t, x, y, z) \approx \Psi_0(t, x, y, z) = \Xi^\zeta(\mathbf{k}; t, x, y, z) \quad (118)$$

on the rhs of Eq. (117), use Eq. (113) for the Green's function, and, omitting closed-channel contributions, infer that

$$\begin{aligned}\lim_{z' \rightarrow z_1+} \Psi(t', x', y', z') &\approx \Xi^\zeta(\mathbf{k}; t', x', y', z_1) \\ &+ \frac{i}{\hbar} \iiint_{B_2} dt dx dy dz \iiint_{\text{open}} d^3 k' \\ &\left[\Xi^B(\mathbf{k}'; t', x', y', z_1) \Xi^B(\mathbf{k}'; t, x, y, z)^\dagger M H_1 \Xi^\zeta(\mathbf{k}; t, x, y, z), \right.\end{aligned}\quad (119)$$

and that

$$\begin{aligned}\lim_{z' \rightarrow z_2-} \Psi(t', x', y', z') &\approx \Xi^\zeta(\mathbf{k}; t', x', y', z_2) \\ &+ \frac{i}{\hbar} \iiint_{B_2} dt dx dy dz \iiint_{\text{open}} d^3 k' \\ &\left[\Xi^F(\mathbf{k}'; t', x', y', z_1) \Xi^F(\mathbf{k}'; t, x, y, z)^\dagger M H_1 \Xi^\zeta(\mathbf{k}; t, x, y, z). \right]\end{aligned}\quad (120)$$

Comparing the above with Eqs. (45) and (53)–(55), we infer that

$$S_o^{\zeta'\zeta}(\mathbf{k}'; \mathbf{k}) \approx \delta^{\zeta'\zeta} I^{\text{open}}(\mathbf{k}' - \mathbf{k}) + i \Delta^{\zeta'\zeta}(\mathbf{k}'; \mathbf{k}), \quad (121)$$

where Δ is the Hermitean matrix

$$\Delta^{\zeta'\zeta}(\mathbf{k}'; \mathbf{k}) = \hbar^{-1} \iiint_{B_2} dt dx dy dz \Xi^{\zeta'}(\mathbf{k}'; t, x, y, z)^\dagger M H_1 \Xi^\zeta(\mathbf{k}; t, x, y, z). \quad (122)$$

Let us now evaluate the dwell times $\tau_D^{II,\zeta}$ for forward ($\zeta = F$) or backward ($\zeta = B$) input. We use Eqs. (75)–(80) with the terms involving the D_2 , the D_4 , and the interference between forward and backward input, all omitted. Substituting Eq. (121), and following an integral by parts, we find that the

terms involving the derivatives of $f_{\text{in}}^\zeta(\mathbf{k})$ cancel, with the results

$$\begin{aligned}\tau_D^{II,F} &= \iiint_{\text{open}} d^3k |f_{\text{in}}^F(\mathbf{k})|^2 \frac{m(z_2 - z_1)}{\hbar k_z} \\ &+ \iiint_{\text{open}} d^3k' \iiint_{\text{open}} d^3k f_{\text{in}}^F(\mathbf{k}')^* \left[\left(\frac{\partial}{\partial k'_t} + \frac{\partial}{\partial k_t} \right) \Delta^{FF}(\mathbf{k}'; \mathbf{k}) \right. \\ &\quad \left. - \frac{mz_2}{i\hbar} \left(\frac{1}{k'_z} - \frac{1}{k_z} \right) \Delta^{FF}(\mathbf{k}'; \mathbf{k}) \right] f_{\text{in}}^F(\mathbf{k}),\end{aligned}\quad (123a)$$

$$\begin{aligned}\tau_D^{II,B} &= \iiint_{\text{open}} d^3k |f_{\text{in}}^B(\mathbf{k})|^2 \frac{m(z_2 - z_1)}{\hbar k_z} \\ &+ \iiint_{\text{open}} d^3k' \iiint_{\text{open}} d^3k f_{\text{in}}^B(\mathbf{k}')^* \left[\left(\frac{\partial}{\partial k'_t} + \frac{\partial}{\partial k_t} \right) \Delta^{BB}(\mathbf{k}'; \mathbf{k}) \right. \\ &\quad \left. + \frac{mz_1}{i\hbar} \left(\frac{1}{k'_z} - \frac{1}{k_z} \right) \Delta^{BB}(\mathbf{k}'; \mathbf{k}) \right] f_{\text{in}}^B(\mathbf{k}).\end{aligned}\quad (123b)$$

It can be shown that both the above times are real.

The reflection coefficients are both first order in H_1 , so the reflected particle current is of second order in H_1 for either type of input—all the particle current is transmitted in the first-order approximation. The mean currents of time upon reflection are also second order in H_1 (see Eqs. (83b) and (86b)). Hence delay times for reflection involve the ratio of two second-order quantities, so that we can obtain at most a kind of zeroth-order approximation to the reflection delay times; each transmission delay time is the same as the respective dwell time to first order in H_1 . To estimate the $B \leftarrow F$ reflection delay times, we substitute the $\zeta' = B, \zeta = F$ block of the approximate S -matrix into Eqs. (81a), (83a), and (83b), and combine the results in Eq. (88b); for the $F \leftarrow B$ reflection delay times, we substitute the $\zeta' = F, \zeta = B$ block of the S -matrix into Eqs. (84a), (86a), and (86b), and combine the results in Eq. (88d).

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